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20. ABSTRACT - Continued

The Joint Services Electronics Program at the Polytechnic is the core of interdisciplinary research in electronics encompassing programs in the departments of Chemistry, Electrical Engineering and Physics under the aegis of the Microwave Research Institute (MRI). The total effort in electronics is coordinated by an MRI Research Committee as a program reflecting evolving techniques and developing faculty interests and expertise in program areas responsive to the scientific and technical needs of the three armed services as represented by the Joint Services Technical Coordinating Committee (JSTCC).

The documentation of research accomplishments during the period of the contract appears in the Progress Reports to the JSTAC (now JSTCC) and in published papers as detailed in comprehensive listings in each of the progress reports. The total impact of the JSEP at the Polytechnic is also evident in the initiation of follow-on research which is continued under separate sponsorship, as well as in the cooperative use of facilities and equipment which have been developed with the continuing support and encouragement of this program under the direction of the JSTCC.

Reports on further progress on each project in the program of research as well as plans for ongoing research and proposed new research projects will be reported upon under the successor contract, F49620-80-C-0077.

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SECTION I: ELECTROMAGNETICS

A. Millimeter Wave Waveguides and Antenna Arrays

S. T. Peng, A. Hessel and A. A. Oliner

1. Objective

To systematically examine the properties of a class of periodically-modulated dielectric waveguides to assess their suitability as scanning antennas for the millimeter wave range. The study would involve first the analysis and measurement of several types of dielectric waveguides suitable for mm wave applications. The results would then be employed in an investigation of periodically-modulated leaky wave structures for use as linear or two-dimensional antenna arrays. These antennas can have a low profile or be flush-mounted, are inherently rugged, are simple to fabricate, and can be made conformal to the surface of a moving vehicle.

This study was initiated in response to interest expressed by the Army, and close cooperation has been continued with new inputs from the user end.

This comprehensive investigation involves the solution of a number of constituent unsolved theoretical problems which are basic in nature and of substantial interest in their own right.

2. Approach

The antennas are viewed as leaky wave structures and are analyzed by considering them as waveguides with a complex propagation constant, the propagation behaviors are determined by microwave network methods. For a systematic and thorough understanding of the wave processes involved, the complex waveguiding problem is broken into simpler constituent ones which are of great theoretical importance in themselves and can be handled independently. The overall waveguiding characteristics are then analyzed in terms of the wave processes associated with each constituent problem. In fact, the computer program for the grating antenna problem will consist of subprograms separately developed for each constituent problem.

3. Progress

Most of the effort during the past year was expended on the part of the program relating to the properties of dielectric waveguides for millimeter waves, since that information is basic to all further work. This effort had three phases. First, approximate results were obtained for a variety of structures using the techniques already developed in the context of integrated optics, and reported in the Renewal Proposal dated 30 September 1978. A notable result found in that study is that, under appropriate conditions, the leakage from the insular waveguide for TE excitation can be extremely high; for one case, a value of α of 4 dB/wavelength was calculated.

Next, after an accurate theoretical solution was obtained and its convergence properties carefully evaluated, it was found unexpectedly that the TE and TM solutions possessed vastly different convergence behavior, with

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with the TE results under good control but the TM ones exhibiting oscillatory convergence characteristics. An examination of the literature showed that this feature had not been quantitatively explored by others; most prior studies dealt only with TE excitation, which produces no problems, and those few which involved TM modes simply assumed that the convergence behavior was similar to that for TE modes. We therefore studied the basic behavior of TM modes for very high values of n , and concluded that a new analytical approach is needed that would minimize the importance of such modes. We have devised such an approach, which greatly improves the situation but which is still under evaluation. Some details of this new approach are presented below. These convergence studies correspond to the second phase mentioned above.

The third phase of the study of dielectric waveguides for millimeter waves was the design and construction of an experimental set-up for measuring the propagation and leakage properties of such waveguides. The first waveguide to be measured will be a form of insular guide, rather than the inverted strip guide, because of our recent discovery that the leakage from insular guides can be very large.

Some further features of the above-mentioned investigations are discussed below. Following these, we describe our progress in connection with grating antennas and then frequency-phase scanning antennas for millimeter waves.

In connection with the approximate techniques mentioned earlier, the dielectric image line, the insular guide, and the inverted strip guide were examined with respect to which modes may leak and which may not. It was determined that none of the modes of the dielectric rectangular image line will leak, but that most modes of the other two structures will indeed leak. For the insular guide, the lowest TM mode is the dominant mode and it will not leak; all of the other modes, including the lowest TE mode, can leak. For the inverted strip guide, the picture is much more involved, in that depending on relative dimensions the lowest TM or the lowest TE mode can leak, but not both simultaneously. The results of this study were presented at a recent symposium,¹ and will appear in a forthcoming paper.²

Approximate values for the leakage from the latter two structures were also evaluated. It was found that the leakage from the inverted strip guide is generally small, but that the insular guide can leak only a little bit or a great deal, depending on circumstances. Under appropriate conditions, the leakage is astonishingly large, and it should be easy to measure.

The third phase mentioned above involved the measurement set-up, which is now well along. The design involves a dielectric ridge waveguide, which is an insular guide with the dielectric constant of the strip equal to that of the layer placed on the ground plane. Careful attention was paid to the feed design, which is always a problem for this class of structures. The waveguide is being excited with the TE mode, obtained from a rectangular waveguide placed on its side. The leakage from the TE mode is TM in nature, meaning that it possesses a vertical element field, so that it can be detected with an ordinary vertical probe arrangement that is designed so that it can be moved either longitudinally or transversely in the horizontal plane. The design is complete and the parts are presently under construction.

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The convergence questions mentioned above absorbed large amounts of our effort because the reliability of the results depends on these very questions. We examined the scattering of waves obliquely incident on a dielectric step junction; even though we took as many as 35 modes on each side of the junction, we found oscillations in the results for the scattering amplitudes, and therefore in the reflection coefficient values, as we slowly increased the number of modes. Such oblique incidence involves the coupling of TE and TM waves. In an attempt to get to the heart of the difficulty, we repeated the calculations for normal incidence, for which the TE and TM waves are decoupled. We found that the convergence for TE waves was reasonably good, but that continued oscillatory behavior was associated with TM mode incidence.

We examined analytically and numerically the modal behavior of TE and TM modes in the limit of very high order modes to assess their effects on convergence. The TE modes behave monotonically but the TM modes exhibit oscillations as mode order n increases. The distinction was traced to the fact that a discontinuity in the field distribution at the air-dielectric interface occurs for TM modes but not for TE modes.

All of the treatments appearing in the literature for wave scattering by a dielectric step hold for normal incidence only. Even there, unfortunately, no satisfactory treatments appear in the literature for TM modes, and, even worse, the problems were usually not even recognized. An exception is Vassalo,³ who pointed out that the scattering by dielectric steps involves very slow convergence, and that his series involved more than 100 terms. The procedure he proposed for improving convergence worked well for metallic discontinuities but, as he shows, not for dielectric steps, leaving the problem unsolved.

In order to assure the reliability of our results, we devised during this past year a new approach to improving the convergence properties. It takes advantage of the asymptotic properties of high order modes, and phrases the analysis so that no inverse of an infinite matrix is needed. Thus, not only is the result more rapidly convergent, but the computer time required is substantially reduced. Since this new approach applies to a large class of dielectric discontinuities, and is of basic importance beyond the type of problem considered here, some of its major features are described below. It is, however, necessary to preface that description with some explanatory material.

We have shown that the modal voltages and currents on the two sides of a step discontinuity between two different dielectric waveguides enclosed by a set of perfectly conducting parallel plates are related by the following set of linear systems of equations:

$$\underline{V} = \underline{Q} \underline{\bar{V}} \tag{1}$$

$$\underline{Q}^T \underline{\bar{I}} = \underline{\bar{I}} \tag{2}$$

where \underline{V} and \underline{I} are infinite column vectors consisting of the modal voltages and currents as their elements, respectively; they will be referred to as the voltage and current vectors. A super-bar is used to indicate a quantity for the transmitted region, in contrast to that without a super-bar for the incident and reflected

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region. \underline{Q} is an infinite matrix characterizing the coupling of modes at the discontinuity. The superscript T indicates the transpose of the matrix. The elements of \underline{Q} are given by the scalar products or overlap integrals of the mode functions on the two sides of the discontinuity as:

$$Q_{mn} = \langle \phi_m(y) | W(y) | \bar{\phi}_n(y) \rangle = \int_0^h \phi_m(y) W(y) \bar{\phi}_n(y) dy \quad (3)$$

where W is a weighting function defined by:

$$W(y) = \begin{cases} 1 & , \quad \text{for TE modes,} \\ 1/\epsilon(y) & , \quad \text{for TM modes.} \end{cases} \quad (4)$$

For the present problem, we assume that the transmitted region extends to infinity so that the transmitted modal voltages and currents are simply related by:

$$\underline{\bar{V}} = \underline{\bar{Z}} \underline{\bar{I}} \quad (5)$$

where $\underline{\bar{Z}}$ is a diagonal matrix consisting of the modal impedances of the transmitted region as its elements. Substituting (5) into (1) and then invoking (2), we obtain:

$$\underline{V} = \underline{Z}^{(in)} \underline{I} \quad (6)$$

where $\underline{Z}^{(in)}$ is the input impedance matrix to the incident waves and is related to $\underline{\bar{Z}}$ by:

$$\underline{Z}^{(in)} = \underline{Q} \underline{\bar{Z}} \underline{Q}^T \quad (7)$$

Thus, the scattering of surface waves by the step discontinuity can now be characterized by the input impedance matrix, as will be done next.

The voltages and currents can be written in terms of the incident and reflected wave amplitudes as:

$$\underline{V} = \underline{Z}(\underline{a} + \underline{b}) \quad (8)$$

$$\underline{I} = \underline{a} - \underline{b} \quad (9)$$

where \underline{Z} is the modal impedance matrix of the incident region, and \underline{a} and \underline{b} are the incident and reflected amplitude vectors, respectively. Substituting (8) and (9) into (6), we obtain

$$(\underline{Z}^{(in)} + \underline{Z}) \underline{b} = (\underline{Z}^{(in)} - \underline{Z}) \underline{a} \quad , \quad (10)$$

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from which the reflected amplitude vector can be determined for a given incident vector. Once \underline{b} is determined for a given \underline{a} , the voltages and currents everywhere can be obtained from (8), (9), (1) and (2), successively. Therefore, the key to the analysis of the scattering of a surface wave by a step discontinuity is the solution of the infinite system of Equations (10). For simplicity, (10) may be written succinctly as:

$$\underline{A}\underline{b} = \underline{c} \quad , \quad (11)$$

with

$$\underline{A} = \underline{Z}^{(in)} + \underline{Z} \quad , \quad (12)$$

$$\underline{c} = (\underline{Z}^{(in)} - \underline{Z})\underline{a} \quad . \quad (13)$$

Equation (11) is an infinite system of linear equations, which has to be truncated for an approximate analysis. For the problem of a step discontinuity between two dielectric waveguides, it is well-known that the method of truncation generally suffers the difficulty of slow convergence. As a consequence, a very large number of modes in each region must be included in an analysis. The inclusion of a large number of modes in such an analysis requires a large computer memory core and long computing time. This reduces the effectiveness of the mode-matching method for dielectric waveguide discontinuity problems. In order to overcome such a numerical difficulty, the estimation of the higher order mode amplitudes based on physical constraints, such as edge conditions on the fields near the discontinuity, has been carried out³ and incorporated into (11), so that only a small number of lower order mode amplitudes are retained for an accurate analysis. However, such an approach was shown to be accurate for metallic diaphragms in parallel plates waveguides, but not for dielectric steps.³

a. New Method

In a systematic study of the modal field distributions at the step discontinuity, we observed that the higher-order modes possess a special property that may be utilized for simplifying the analysis of the key-infinite system of Equations (11). Specifically, (11) may be partitioned in the following manner:

$$\left(\begin{array}{ccc|ccc} a_{11} & \dots & a_{1n} & a_{1,n+1} & \dots & \\ \vdots & & \vdots & \vdots & & \\ \vdots & & \vdots & \vdots & & \\ \vdots & & \vdots & \vdots & & \\ a_{n1} & \dots & a_{n+1} & a_{n,n+1} & \dots & \\ \hline a_{n+1,1} & \dots & a_{n+1,n} & a_{n+1,n+1} & \dots & \\ \vdots & \vdots & \vdots & \vdots & & \\ \vdots & \vdots & \vdots & \vdots & & \end{array} \right) \left(\begin{array}{c} b_1 \\ \vdots \\ \vdots \\ b_n \\ \vdots \\ b_{n+1} \end{array} \right) = \left(\begin{array}{c} c_1 \\ \vdots \\ \vdots \\ c_n \\ \vdots \\ c_{n+1} \end{array} \right) \quad (14)$$

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which may be written as:

$$A_{11}\underline{b}' + A_{12}\underline{b}'' = \underline{c}' \quad (15)$$

$$A_{21}\underline{b}' + A_{22}\underline{b}'' = \underline{c}'' \quad (16)$$

where A_{11} is an $n \times n$ matrix, A_{12} is an $n \times \infty$ matrix, A_{21} is an $\infty \times n$ matrix, and A_{22} is an $\infty \times \infty$ matrix. \underline{b}' and \underline{c}' are n -column vectors and \underline{b}'' and \underline{c}'' are infinite column vectors. The estimate of the higher-order mode amplitudes involves an optimum choice of \underline{b}'' . In contrast to the use of edge conditions on the fields to determine \underline{b}'' , we may obtain directly from (16):

$$\underline{b}'' = A_{22}^{-1} \underline{c}'' - A_{22}^{-1} A_{21} \underline{b}' \quad (17)$$

Substituting (17) into (15), we further obtain

$$(A_{11} - A_{12} A_{22}^{-1} A_{21}) \underline{b}' = \underline{c}' = -A_{12} A_{22}^{-1} \underline{c}'' \quad (18)$$

which is a finite system of equations. It is emphasized that although only the lower-order reflected mode amplitudes appear in the equation, (18) is an exact one that takes into account the effect of the higher-order modes. Unfortunately, A_{22} is an infinite matrix whose inverse, A_{22}^{-1} , is difficult to determine. However, for the dielectric step discontinuities, we observe that A_{22} possesses the special property:

$$A_{22} = D(1 + S) \quad (19)$$

where D is a diagonal matrix, 1 is a unit matrix and S is a matrix without diagonal elements such that its norm is much smaller than unity, e.g.,

$$\|S\| \ll 1 \quad (20)$$

Therefore, the inverse of A_{22} can be approximated as:

$$A_{22}^{-1} = (1+S)^{-1} D^{-1} \approx (1-S) D^{-1} \quad (21)$$

With such an approximation for (18), the lower order reflected mode amplitudes can now be easily determined, including the effect of the higher-order modes.

The utility of this new approach is presently under investigation. It works beautifully and rapidly for TE modes, as expected. Its application to TM modes certainly improves the convergence behavior, but the number of modes needed for a specified accuracy is currently under examination. When the study relating to normal incidence is completed, the method will be extended to the oblique incidence case, for which the TE and TM modes become coupled. Then, after the scattering problems, which are of interest in themselves, are

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satisfactorily understood, the calculation procedure will be adapted to the case of waveguide guidance, which was our original goal. The convergence difficulties encountered were not expected to the extent found, but they uncovered a basic problem which led to a new approach to the question of convergence improvement.

The next area of work involves grating antennas suitable for millimeter waves. It is well understood that a grating antenna structure of finite width is a three-dimensional boundary value problem that supports only hybrid modes, i.e., it requires simultaneous presence of "TE" and "TM" waves in the structure. To our best knowledge, no attempt has ever been made in the literature to formulate a periodic dielectric waveguide for the general case of oblique guidance, possibly because of its mathematical complexity and lack of practical interest in the past. For the analysis of grating antenna structures of finite width, however, a satisfactory analytical (not simply numerical) treatment of the general case becomes a necessity. For the case of normal incidence, the grating antenna structure has been successfully formulated in an exact fashion and without any restriction condition.⁴ The formulation is carried out in terms of both sets of TE and TM Floquet mode functions of the periodic tooth region. Each of these sets of mode functions has separately been analyzed extensively in the previous formulation for the special case of normal guidance where the TE and TM modes are decoupled.

An exact formulation for the general case of oblique incidence has been recently reported.⁴ In carrying that work further, we have, as proposed, successfully carried out during the past year the development of a computer program based on the exact formulation for the general case that will account for the effect of lateral variations of electromagnetic fields on the radiation characteristics of a grating antenna.

In the development of the computer program for the grating antenna under the most general conditions, we have adapted an approach that is well-known in microwave engineering. Namely, we divide a complex problem into several constituent problems which may be individually analyzed in an exact fashion to identify and to understand basic physical processes that may occur. The physical phenomena associated with the composite structure may then be analyzed conveniently in terms of the well understood basic physical processes involved. Since scattering of a plane wave by a periodic layer is the basis for the radiation of a grating antenna, it is essential to solve the scattering problem first. Also, the scattering problem is of fundamental importance by itself. Therefore, we have first developed a computer program for the plane wave scattering by a periodic layer. With this program, extensive numerical results have been obtained, showing the coupling of power between TE and TM modes. This represents the first successful analysis of a three-dimensional vector boundary value problem involving a periodic structure. The computer program developed can be said to be the most general one for the grating antenna structure and is expected to have a great impact on future research on the subject.

Our program on new dielectric antennas suitable for the millimeter wave range also includes the analysis of steerable phase-frequency corrugated planar arrays.

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Phase-frequency steerable arrays are envisioned as low cost substitutes for the considerably more expensive and more customary phase-phase scanning planar arrays. The antennas under investigation consist of a periodic arrangement of leaky-wave line sources. Each such traveling-wave subarray consists of a grounded dielectric strip periodically loaded with rectangular grooves (corrugations). The beam is frequency scanned in the principal plane of the line source and phase-scanned in the orthogonal plane.

The first step in the analysis is the determination of modes of propagation in an infinitely-extended dielectric-rodded medium with rods having a rectangular cross section. To this end, a computer program for propagation along an infinite periodic stack of parallel dielectric slabs is being developed, when the phasing along the direction of periodicity and along a direction orthogonal to that of the periodicity is imposed. This procedure generalizes the results of Lewis and Hessel⁵ in which the latter phase gradient is zero. The analysis is simplified by recognizing, as in Reference 5, that the TE and TM modes are uncoupled with respect to the normal to the dielectric slab.

After establishing the dispersion relation and the fields for the stack of parallel dielectric slabs, we intend to apply Galerkin's procedure to the determination of discontinuities in a periodically interrupted set of dielectric slabs, which in turn lead to the dispersion relation for the rodded medium.

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B. Hybrid Ray-Mode Formulation of Ducted Propagation

L. B. Felsen

1. Objective

Ray optical and guided mode expansions have been used as alternative methods for analyzing high-frequency propagation in layers and ducts. When the waveguide boundaries are penetrable, the discrete spectrum of guided modes is generally augmented by a continuous spectrum. In ducts of large cross section compared to the operating wavelength, the number of trapped modes may be exceedingly large so that truncation of the mode series has frequently been implemented, and the continuous spectrum ignored. Alternatively, ray models may require a very large number of reflected or refracted rays so that the "ray series" is terminated at some finite limit. Criteria justifying the truncation and assessing the resulting error have generated in this fashion may therefore be open to question.

In view of these observations, it is desirable to develop a systematic procedure that can account for the remainder of a truncated ray or mode series. A properly-chosen, range-dependent combination of rays and modes would not only furnish an accurate and convenient field representation, but would also provide new basic insight into the propagation process.

Our objective is to develop a new and systematic procedure that can account for the remainder of a truncated ray or mode series, and thus improve the accuracy of the field representation for high frequency propagation in layers and ducts. This is to be accomplished with a properly-chosen range-dependent combination of rays and modes, which also should provide new basic insight into the propagation process.

2. Approach

Field representation for propagation in layers and ducts in the high frequency range, where the field is generally characterized by very many rays or very many modes, will be determined by means of a suitably chosen mixture or both rays and modes in order to produce a more convergent and more accurate formulation.

3. Progress

During the past year, the hybrid ray-mode results for source-excited circular cylindrical concave surfaces have been transformed into corresponding results for propagation in a surface duct generated by a refractive index profile that decreases exponentially away from the surface. The correspondence is established directly by mapping the cylindrical boundary into a plane boundary.¹ Having thus gained an understanding of how to construct effective ray-mode combinations for this special case, we generalized the procedure to accommodate surface ducts with arbitrary (but slow) monotonic refractive index profiles.¹ As for the concave boundary,²⁻⁴ the ray-mode mixture is far more efficient than a formulation involving only rays or only modes. It accounts, furthermore, for the cumulative effects of rays with many surface reflections.

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Such ray fields cannot legitimately be treated by ray optical methods since they do not satisfy the local plane wave requirement.

In the above example, the duct boundary was taken to be perfectly reflecting or describable by a surface impedance. A more general situation arises when the boundary separates two media with different refractive indices. Since the boundary is now penetrable, the surface trapped mode or ray fields may become leaky and lose energy either by evanescent tunneling or by refraction into the exterior medium. Such a situation arises in an elevated tropospheric duct where guiding occurs along a small discontinuous change in the refractive index of the atmosphere.⁵ For source and observation point locations on the duct boundary, we have calculated the beyond-the-horizon field by the hybrid ray-mode technique and have compared the results with solutions generated by direct summation of the normal modes. Again, the hybrid method substantially improves the efficiency of the numerical computations, and it grants some basic new insights into the propagation process.

In the investigations described above, the source and observation points were both located on the duct boundary. We shall now explore the modification of the hybrid formulation when the source point and/or the observation point are removed from the boundary and situated either within or outside the duct region. It is anticipated that ray optics alone can then provide an adequate description of the field since the "non-permissible" rays with many surface reflections do not now arrive at the observation point. The question of how to deal most effectively with the field near the various reflected ray caustics will also be considered.

A major modification of the hybrid procedure occurs when ducting is caused not solely by an appropriate refractive index inhomogeneity but by multiple reflection between two boundaries. Preliminary investigation shows that a few near cutoff waveguide modes can represent the cumulative effect of ray fields that have undergone many reflections between the waveguide walls. To ascertain the basic field behavior in a simple canonical configuration, we shall study in detail hybrid ray-mode representations of the parallel plane waveguide Green's functions.

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C. Wave-Matter Interactions

S. Barone, S. Gross and N. Marcuvitz

1. Objective

Our objective is to extend to nonlinear and/or higher power levels and to develop, both theoretically and experimentally, engineering expressions for "collision" (interaction) terms necessary in the description of particle-particle, particle-wave and wave-wave interaction problems arising in electromagnetic wave propagation through media in which ionization and related phenomena arise. The latter include microwave breakdown processes associated with high power wave propagation thru the atmosphere, microwave propagation thru and modification of the ionosphere, plasma screening effects in laser wave absorption and reflection by materials, etc.

2. Approach

An overall analytical theme is to obtain a kinetic basis for models of "collisional" interactions. Kinetic models must be consistent with the rate equations and the experimental rate coefficients and must provide reasonably correct representations of physical phenomena both at the kinetic and fluid levels. For example, a possible general form for the kinetic equation describing the density distribution function $f_a(v, r, t)$ of particles of type "a" from which fluid equations may be derived is:

$$\frac{d}{dt} f_a = \nabla_v \cdot \underline{\underline{D}} \cdot \nabla_v f_a + \nabla_v \cdot \underline{\underline{A}} f_a + C_a(f_1, f_2 \dots)$$

where $\underline{\underline{D}}$ and $\underline{\underline{A}}$ are diffusion and friction coefficients indicative of long range (particle-wave) collisions and C_a is indicative of short range collisions. While it is also possible to include some short range (particle-particle) collisional contributions in $\underline{\underline{D}}$ and $\underline{\underline{A}}$, others involving transfer of non-infinitesimal amounts of energy and non-particle conserving collisions, such as ionization and recombination, must be included in the C_a term. Our initial collisional models are suitable only for kinetic equations that are isotropic in velocity or energy. However, in the presence of large applied electric fields the isotropy assumption has limited validity particularly when electron velocities are larger than the thermal speed. The use of the microscopic kinetic approach of Klimontovich, together with renormalization and quasiparticle techniques,^{1, 2} are being explored to remove the isotropy limitation. Moment of fluid equations derived from such kinetic models will be checked for consistency with experimentally determined momentum, energy transfer, ionization, etc., rates. The sensitivity

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of kinetic and/or fluid descriptions to various collisional models will be studied by developing and comparing analytical and numerical models of overall physical processes on our interactive graphic computer facility.

3. Progress

The isotropic electron kinetic equation with collisions has been employed to refine the electron density and energy equations in our model of high power microwave propagation in the presence of atmospheric breakdown. A concomitant kinetic equation has been used for the quasiparticle description of the electromagnetic field. These studies have contributed to what is regarded as the first self-consistent, space-time detailed model of the propagation of a microwave pulse with tail erosion from atmospheric breakdown. To validate the model, we are carrying out, with additional ONR and NRL support, a series of measurements at pulse microwave power densities of kilowatts/cm² in a partially-evacuated S-band waveguide. As indicated in Fig. 1, the pulse shortening observed for a 100 ns pulse for guide pressures of 0.5 to 6 Torr is in good agreement with the computer model results and therefore does validate the model for these low power density and low field strength conditions. We are planning to make high-power measurements at megawatt/cm² pulse intensities using the new gigawatt magnetron at NRL.

Preliminary calculations of kinetic distribution functions for electrons including excitation and de-excitation processes have been completed. Our current lack of local graphic 32-bit computational facilities is hindering the inclusion of ionizing collisions in such studies.

Our kinetic studies have been applied to a fluid dynamic model of laser induced melting,³ vaporization,^{4, 5} and breakdown of material evaporated from an irradiated target at approximately 10⁷-10⁹ watts/cm². The space-time evolution of the parameters in the "blow-off" plasma have been studied analytically and numerically in a time scale short compared to that required for significant fluid motion. Our studies went beyond some recent related work of R. J. Harrach (Laser Livermore Laboratory) in that spatial variations were considered. Also, in contrast to some earlier studies by Bergelson (USSR) it was shown that the conditions for Saha equilibrium are not applicable.

Our studies of nonlinear fluid dynamic wave-wave interactions has led to a new approach⁶ to some ionospheric irregularity problems and has been applied to the nonlinear development of the gradient-drift instability in the equatorial E-region;^{7, 8, 9} it has also been extended to the Rayleigh-Taylor instability on the bottom side of the equatorial F-layer. The former is responsible for type II irregularities and the latter is believed to be an important factor in equatorial spread F. We have studied the E-region problem numerically for both quadratic and cubic nonlinearities and analytically via the direct interaction approximation for the full nonlinearity to all orders. Possible reasons for the qualitatively different results obtained have been explored. In the F-region problem, we have obtained results for both small scale fluctuations and large scale density depletions (bubbles). The small scale fluctuations can be discussed within a quadratic theory, but the understanding of large scale depletions requires the full theory. We have also

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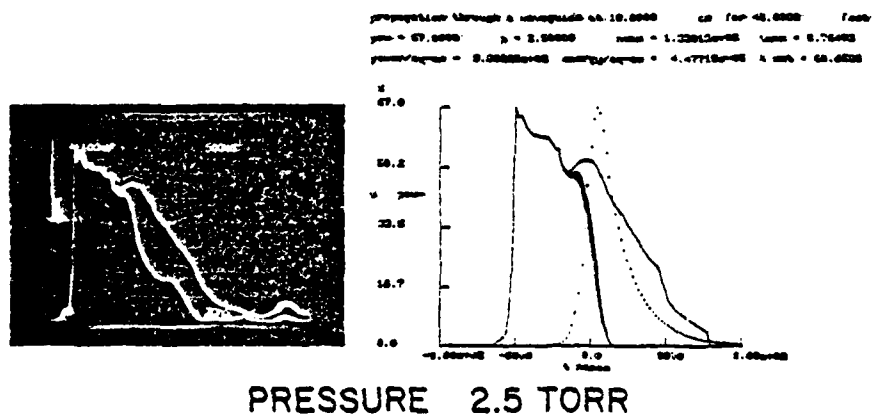
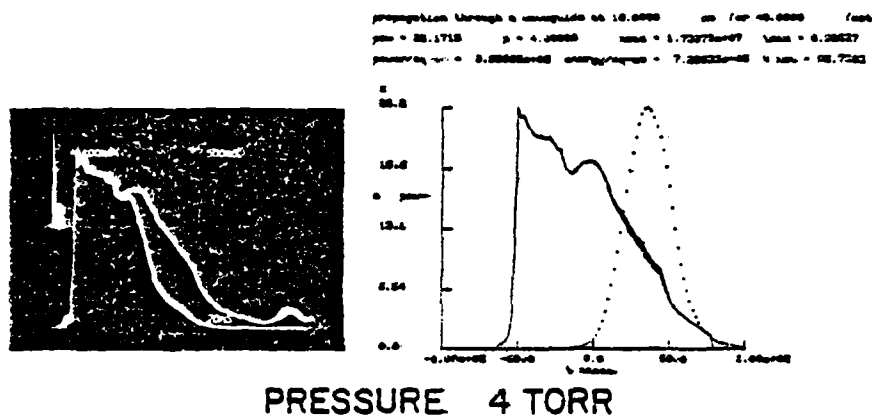
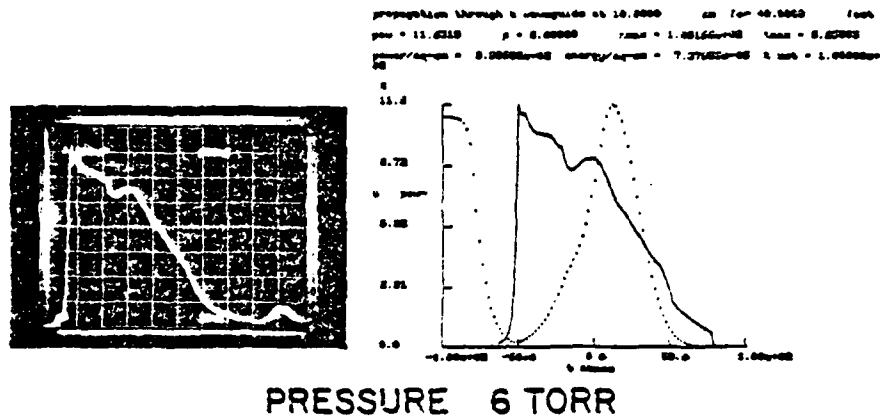


Fig. 1. Comparison of experiment with computer model results for propagation of a microwave pulse in a partially-evacuated waveguide.

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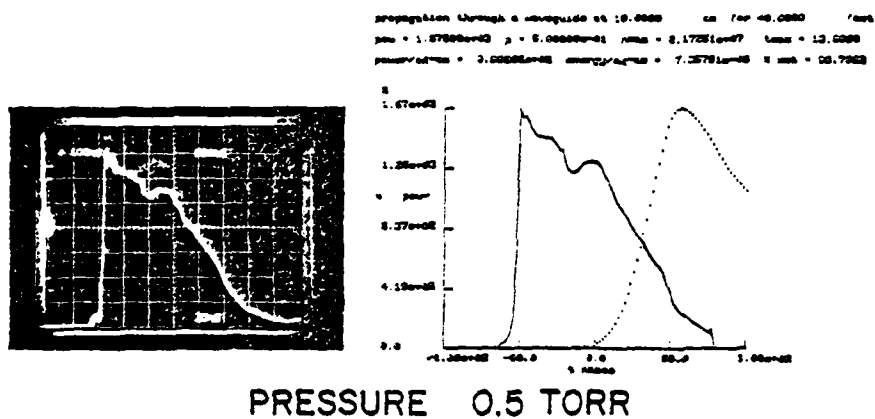
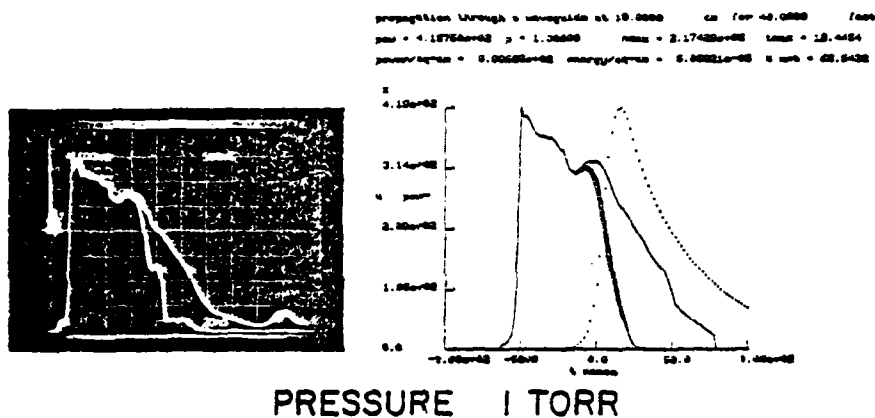
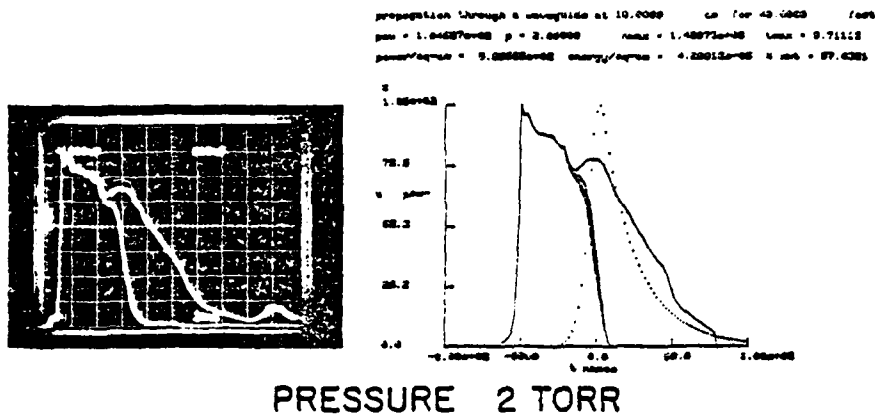


Fig. 1 (Cont). Comparison of experiment with computer model results for propagation of a microwave pulse in a partially-evacuated waveguide.

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developed a new point of view towards anomalous nonlinear interaction terms (enhanced diffusion, anomalous resistivity) in the plasma content.¹⁰ This approach goes beyond previous theories in that it suggests a technique for discussing anomalous interactions independent of perturbation theory.

In accordance with the kinetic equation noted in Section C.2, a self-consistent evaluation of the diffusion coefficient has been used to analyze the stabilization of parametric instabilities in the quasi-linear regime due to heating effects.^{11, 12} Phenomena of hysteresis and overshoot of excited instabilities observed in ionospheric modification experiments can be explained. The classical technique of transformation and characteristics was developed to analyze^{14, 15} strong plasma turbulence. Diffusion coefficients for both homogeneous and inhomogeneous media were obtained to all orders without time singularities. A bulk heating diffusion coefficient has been found.¹⁶ It is shown that when the pump field is of the order $E_0 \geq (4\pi n_0 T_e)^{1/2}$, significant bulk heating can be present.

Measurement of specular and total reflectances of metal surfaces during intense pulsed laser irradiation¹⁷ has continued with additional support from AFOSR and ONR. Papers describing the reflectance behavior, surface temperature history, and the nature of the metal surface changes have been presented at several meetings.^{18, 19, 20, 21} When the incident laser power intensity exceeds $\sim 2 \times 10^8$ watts/cm², a "light flash" is observed. The light flash can be misinterpreted as a recovery of the target surface reflectance if the detection system does not include narrow band detection at the laser wavelength. The nature of the "light flash" is being examined. Refinement of the total reflectance measurements is now beginning to reveal differences in the reflectance behavior for different target surface material preparations, for example, between vacuum deposited copper surfaces which have been vacuum annealed and those which have not. A probe laser is being installed both to measure reflectances over a longer time interval as well as to simultaneously measure at a second wavelength and look for nonlinear effects.

Quasiparticle descriptions of wave propagation in inhomogeneous and nonlinear media supporting wave-wave interactions have been studied both analytically and numerically. A number of kinetically based numerical algorithms have been evolved for such problems, the accuracy of the quasiparticle approximation has been evaluated for several cases, and a comparison of the (caustic free) quasiparticle method with various ray techniques have been developed.

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D. Optical Waveguiding Structures

T. Tamir, A. A. Oliner and L. B. Felsen

1. Objective

- (a) To investigate the waveguiding and coupling properties of dielectric gratings having asymmetric (blazed) profiles for applications to beam couplers, filters, distributed-feedback lasers and other integrated-optics components. In particular, criteria for the design of high efficiency gratings having prescribed desirable characteristics will be studied.
- (b) To analyze and characterize the behavior of basic discontinuity structures found in integrated-optical circuits, to determine their reflection and scattering characteristics. No one has yet performed such analyses to any degree of accuracy. The simple dielectric step junction will be examined first. It will be analyzed rigorously, and then to varying degrees of approximation, determining the simplest form suitable for recommendation.
- (c) To analyze the propagation characteristics of various linear (strip-type) waveguides of importance in integrated-optical circuitry. Such waveguides have so far been analyzed by others only to first order. A better analysis has already revealed the presence in some waveguides of leakage and resonance effects which were heretofore unrecognized and which could have important device implications. Several different

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types of waveguide will be examined, and to various degrees of accuracy. The results obtained under (b) above for the dielectric step junction (since the sides of strip waveguides correspond to such junctions) will be applied in this connection, particularly those results which include the continuous spectrum contributions.

- (d) To analyze the propagation characteristics of various diffused channel guides of importance in integrated-optical circuitry. Since the boundaries of such guides are not rectilinear (as they are for most strip guides), nor usually uniform in the refractive index distribution, the customary analytical methods are not applicable. We are developing an approximate analytical method which utilizes the dielectric step junction results of (b) above. The results obtained for the waveguide characteristics will be compared, where possible, with available finite-element numerical calculations and with experimental data. This project is completely new to this program
- (e) To analyze the properties of a novel leaky-wave optical directional coupler. This directional coupler consists of two parallel strip waveguides which are subject to the leakage property mentioned under (c), and are separated sufficiently so that the only coupling between them can occur via leakage. This coupling structure will serve first to verify quantitatively the importance of the leakage effects which the waveguide analysis has revealed. In addition, the coupler may indeed yield a practical device because its dimensional tolerances seem to be much less demanding than those of customary couplers, and because it can serve as a novel mode-stripper which eliminates the "TM" mode content of the guided wave and produces pure "TE" propagation.
- (f) To examine analytically the properties and the implications of a newly-recognized total absorption effect associated with thin lossy layers and with metallic periodic structures which are not perfectly conducting. Recent work has shown¹⁻³ that, if electromagnetic energy is incident on a planar structure consisting of a thin lossy layer and/or a metallic grating, all or nearly all of the incident energy can be absorbed by properly adjusting the incidence angle and the dimensions of the planar structure. The interesting aspect of this effect is that total absorption can be realized without the need for thick lossy absorbers. The aim of the proposed work is to first examine the total-absorption effect in detail for both layered media and periodic (grating) structures and then to apply the results to a variety of applications, which include the design of PN photodiodes having both quantum efficiencies and very rapid response characteristics. Other applications of the total absorption effect (e.g., for non-destructive evaluation of materials, for reducing the cross-section of radar targets, etc.) will be explored later.
- (g) To explore a new asymptotic theory for propagation in guiding regions with inhomogeneous permittivity properties. The results are expected to be relevant for integrated-optical and optical fiber waveguides, underwater sound wave propagation in the ocean, ducting in

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the ionosphere, and related applications. This theory will be applied to various graded-index waveguides, including both slabs and fibers, with a view toward accommodating analytical refractive index profiles of arbitrary shape. Such structures would include profiles with discontinuous changes in the index or its derivatives; the theory will later be generalized to waveguides with asymmetrical boundaries, with longitudinal variation, and with curved axes.

2. Approach

The approaches used in the various aspects of this program employ a number of theoretical techniques that have already been developed to a high degree of sophistication and success in the area of microwave engineering. In particular, the researchers on this program have personally contributed significantly to the development of these techniques, which include transverse resonance methods, various approximate and rigorous modal methods, and periodic structure theory. In most aspects of the program, the theoretical techniques themselves are developed further in the course of the investigations. This is especially true in connection with the investigations relating to graded-index guiding structures, where a new method embodying local evanescent fields with complex phase is employed, instead of the conventional asymptotic theories which utilize local ray fields or mode fields with real phase.

Experimental checks will be employed in limited aspects of this program, either by direct optical measurements, by modeling at millimeter wavelengths, or by cooperating with industry (e.g., Bell Laboratories).

3. Progress

(a) Dielectric Gratings for Integrated Optics

In connection with the study on dielectric gratings for integrated optics applications, we had in the past developed a rigorous solution⁴ of the pertinent boundary-value problem, which yields highly accurate results for the fields scattered and/or guided by dielectric gratings. In addition, we obtained a simpler perturbation solution⁵ of the same problem, which is accurate enough for many practical purposes. Most recently, we have developed a novel Bragg-reflection interpretation,⁶ which yields an excellent qualitative and a very good quantitative description of the scattering properties of dielectric gratings. Basically, the Bragg-reflection approach looks at the gratings in terms of an extended two-dimensional periodic lattice structure which is used to predict the preferred directions of scattered energy. This approach provides a simple interpretation of both scattering and coupling to guided waves, which has been found to be especially useful for the design of blazed gratings for high-efficiency couplers.^{7,8}

Based on the above techniques, the operation of gratings having symmetrical profiles has been examined in detail. In particular, the performance of beam couplers constructed with symmetrical gratings has been investigated in depth and accurate design criteria have been developed.⁹ However, gratings having asymmetrical profiles offer interesting directional properties, which

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cannot be achieved by means of symmetric gratings. In particular, by blazing the grating profile, it is possible to suppress scattering in undesirable directions and thus to enhance the efficiency of beam couplers. We have, therefore, concentrated during the past year on efforts to confirm preliminary results⁶ dealing with this desirable blazing effect. In particular, our study has included the following efforts:

- (1) We have developed a simple design criteria for constructing a blazed grating having an asymmetrical triangular profile, which can achieve nearly 100% efficiency by coupling energy into the preferred direction. In addition, we have examined the effects produced by departures from the ideal triangular shape and we have found that tolerances and other fabrication constraints are not critical. Other grating profiles, such as trapezoidal and rectangular shapes, have also been examined in this context.
- (2) To verify the conclusions reached under item (1) above, an optical grating was modeled (scaled up) to the x-band microwave region by using a teflon grating inside a parallel-plate set-up. The design was based on an optimized asymmetric triangular grating profile which was calculated to offer a theoretical efficiency of 98%. The scaled-up model was constructed and preliminary measurements showing an efficiency of 96% have been already confirmed. Other measurements, which involve the parameters of the leaky-wave supported by the grating, have also shown a very good agreement between the theoretically predicted values and the measured data.

The results of the past year's work have been reported at an NSF meeting,¹⁰ and a paper dealing with item (1) is being processed for publication.¹¹ The work described in item (2) is to be continued throughout the next year with the intention of developing further the approach of modeling optical dielectric gratings at microwave frequencies. This microwave modeling approach makes it possible to investigate grating properties that are very difficult to study at optical wavelengths because of either fabrication or measurement difficulties.

(b) Scattering Properties of Basic Discontinuity Structures

The dielectric step junction is the discontinuity structure to be studied first because it corresponds to the side wall of dielectric strip waveguides and because it occurs as an integral element of other structures for integrated optics applications, such as multiplexers and modulators. We have been examining both approximate and rigorous analytical formulations in this context.

It has been widely recognized that the equivalent dielectric constant method yields a very simple result for the reflection coefficient of a surface wave incident on a dielectric step junction. The procedure assumes that the regions on each side of the junction can be represented by an equivalent (or effective) dielectric constant, and that the junction discontinuity then reduces to a simple interface between two dielectric media. The geometrical discontinuity then excites no higher modes. As a result, the approach cannot yield information on any radiation scattering, but good values in very simple form are found for the reflection and transmission coefficients of the surface wave.

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During this past year, a careful examination was conducted on why this approximate approach yields such good results despite the brashness of the approximation (throwing away the geometric nature of the junction). It was found that the same result is obtained if the geometry of the junction is retained, and if the field in the junction plane is taken to be the average of the surface wave fields on each side of the junction. Such a field assumption is very reasonable, and is certainly better than the usual ones which are taken for overlap integral approximations, namely, the surface wave field on one side or on the other of the junction. Besides explaining why the equivalent dielectric constant procedure works as well as it does, the above recognition thus offers a systematic procedure for improving various approximation schemes involving overlap integrals.

The equivalent dielectric constant approach is applicable only when one mode is present on each side of the junction. For oblique incidence, when TE and TM modes couple to each other, this direct approach is inadequate. However, the recognition above involving the average field can be applied to such coupled situations, and should offer a simple yet accurate approximation. Expressions for the scattering coefficients for the oblique incidence cases are being developed currently; numerical values obtained from them will be compared with those found from more accurate calculations involving many modes.

Calculations were made during the past year for the scattering by a dielectric step junction on a substrate using a rigorous phrasing based on the discretization of the continuous spectrum.¹² In order to obtain numerical results from this rigorous phrasing, which takes all modes into account, it is necessary to truncate the infinite matrices which are present, and effectively to account for only a finite number of modes. From previously-published accounts, which apply only to normal incidence (so that the TE and TM modes are decoupled) and usually to TE modes only, we were led to expect satisfactory convergence behavior when the modal series were truncated. We found instead that, as the number of modes taken into account was increased, the results showed oscillatory behavior rather than the monotonically-decreasing behavior we were led to expect.

These unexpected convergence difficulties occurred also for corresponding dielectric structures in our millimeter waves study (reported on pages 1-8 of this report). As described there in greater detail, these observations led to a systematic inquiry into the causes of the poor convergence (the TM modes exhibit the difficulty but the TE modes do not), and to the development of a new treatment for the modal expansions which exploits a special property of very high order modes and yields numerical results which are more rapidly convergent. This new approach is described in the millimeter wave study, and is currently under evaluation numerically. When its utility is satisfactorily understood, it will be applied to the class of structures discussed above. It is expected that this will occur soon.

(c) Leakage Characteristics of Dielectric Strip Waveguides

Our studies on the propagation properties of three-dimensional dielectric waveguides for integrated optics have revealed that such structures permit the existence of a new class of leaky modes. We were the first to demonstrate

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that certain modes on such waveguides can indeed leak energy, and thus produce cross talk between neighboring components on the same substrate. Since then, we have explored in general terms the leakage properties of various mode types on a number of such waveguides. These general studies are summarized in a forthcoming paper.¹³ One novel general property of this new class of leaky modes is that the polarization of the leakage energy is opposite to that of the bulk of the energy guided by the waveguide itself. For example, if a strip waveguide is excited with TM polarization, the leakage from this mode is in the form of a TE surface wave in the surrounding layered region.

A second publication in process¹⁴ relates to a simple method for predicting leaky waves on rib waveguides, which are strip guides for which the refractive index of the strip is the same as that of the layer. This method is a refinement of the one described in last year's proposal, but is also based principally on the dispersion plots for the surface waves in each region independently.

During the past year, we obtained more accurate numerical values for the attenuation constants of some leaky modes on dielectric strip waveguides. Previously, our numerical values¹⁷ were based on the presence of the various coupled TE and TM surface waves only, and the continuous spectrum was neglected. The new calculations account for the continuous spectrum by using the discretized procedure described in last year's proposal. Mittra et al.¹⁵ have also used this approach for dielectric waveguides, but regrettably they admit they never looked for complex values, and they therefore missed entirely the only interesting new feature of these solutions, that of leakage.

Numerical values obtained from this more accurate theoretical procedure show that the earlier approximate values were in general about 1.5 to 2 times too large, but that they nevertheless formed a good guide to the magnitudes of leakage involved. A paper by Japanese authors recently appeared¹⁶ which observed that our published results¹⁷ neglected the continuous spectrum; they then presented results based on an approximate method for taking the continuous spectrum into account. Numerical values obtained by them were superimposed on our published plotted data in Reference 16, and the Japanese authors concluded that our approximate data were too small by an order of magnitude. Since our later, more accurate, results yielded smaller values than the approximate ones, whereas these authors found larger values, we were puzzled. We concluded tentatively that something must be wrong with their development. Recently, however, these Japanese authors kindly informed us that they found a numerical error in their results, and that they will submit a correction to Applied Optics. Their published values, which were about 10 times larger than our approximate values, are in error by a factor of $(1.6\pi)^2$, which is about 25. Their modified values now turn out to be rather close to our new, more accurate, values which is rather gratifying.

Because of the convergence problems mentioned in (b) for the scattering by a dielectric step, we have suspended further calculations of the leakage effects. Even though the guided wave propagation constants are less sensitive than the scattering results to errors due to poor convergence, numerical errors may exert an important influence for certain parameter ranges, especially for α . We feel it would be prudent to first settle the convergence

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questions, and then complete the calculations of the leaky wave properties.

(d) Study of Inhomogeneous Channel Waveguides

This study was not scheduled to begin until next year.

(e) Novel Leaky-Wave Directional Coupler

An examination of the properties of this class of structures was to follow the completion of the calculations on the leakage properties of single strip waveguides. Since, as described under (c), such calculations will be completed after the convergence questions are satisfactorily settled, the directional coupler study is being postponed temporarily.

(f) Anomalous Absorption Effects in Multilayered and Periodic Structures

Most of the work carried out by others so far on total absorption by thin, slightly lossy, planar structures has regarded this phenomenon as either an anomalous behavior, which was verified in metallic gratings by intricate computer calculations,¹ or as energy coupling to an electron plasma wave, which occurs for only TM modes in the presence of a metallic conductor.² However, we have been able to show³ that the total-absorption phenomenon is due to a leaky-wave mechanism, which may occur for both TM and TE waves. Furthermore, the small loss mechanism required to produce total absorption of the incident wave need not involve metallic conductors and may, instead, appear also if dielectric losses are present in thin (non-periodic) layers.

During the past year, we have further developed our preliminary results³ for multilayered media, but the emphasis has shifted to periodic structures. The analysis of the latter is much more complicated and requires the accurate calculation of the scattered waves. We have, therefore, examined this problem by using the following two approaches, which have been studied in parallel.

1. A previous idealized but simple model¹⁸ for lossless gratings has been extended by us¹⁹ to examine lossy gratings. This has provided considerable insight into the scattering effects produced by absorption anomalies.
2. A highly accurate method based on an exact solution previously developed by us⁴ for studying waves guided by a lossless dielectric grating was extended to evaluate waves scattered by lossy gratings having arbitrary profiles, which can be of either dielectric or metallic varieties or a combination of both. Results obtained by this very general technique have confirmed the validity of the simple model described in item 1; our approach will facilitate the derivation of an even broadened spectrum of useful results for waves scattered or guided by gratings, of which absorption anomalies form only one of several applications.

A particularly useful result of the two items 1 and 2 above is that they are applicable to both perpendicular (TE-mode) and parallel (TM-mode) polarizations of the incident fields, in contrast to recent work by others,^{20,21} which was restricted to the former polarization. This is important not only from an

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analytical point of view. Phenomenologically, plasmon waves are supported only in the case of TM modes over lossy metallic structures, so that the extension of our results to parallel polarization is essential for their study. A paper on this subject is presently being completed for publication.²²

(g) Propagation in Inhomogeneous Media Using Local Evanescent Fields

During the past year, the evanescent wave method for propagation in slab and fiber waveguides with analytic graded index has been put on a firm foundation. As formulated originally,^{23,24} it was assumed that the asymptotic expansion coefficients A_n of the modal field amplitudes A in inverse powers of the large wavenumber k must be analytic on the waveguide axis because the rigorous mode solution is known to be analytic there. Enforcing this condition permitted the self-consistent determination of the asymptotic expansion coefficients β_n for the modal propagation constant β and hence for the modal group delay. However, the analyticity assumption for the A_n was of questionable validity since the asymptotic expansion becomes singular as the observation point approaches the axis.²³ Nevertheless, the asymptotic expansion for β determined in this manner agreed term-by-term with those of available exact solutions, and this circumstance was regarded as a justification of the procedure. Moreover, it was shown¹ that the singular terms near the axis could be isolated and expressed in closed finite form in terms of the canonical Hermite or Laguerre polynomial solution for a parabolic index profile in two and three dimensions, respectively.

In collaboration with Dr. J. Arnold (Electrical Engineering Department, University of Nottingham, England), who was also bothered by the assumption in Reference 23, we have now been able to provide a rigorous basis for the Choudary-Felsen procedure.²⁵ We have shown that the asymptotic expansion coefficients A_n must be single-valued in a strip of the complex transverse coordinate plane. This requirement has precisely the same effect as the improperly imposed analyticity condition. Thus, it is no longer necessary to justify the correctness of the asymptotic expansions for the modal amplitude A or the propagation constant β in slab or fiber waveguides with analytic graded index by comparison with exact solutions for special profiles.

Some progress has also been made in the analysis of slab waveguides with refractive index that varies transversely and longitudinally with the weak longitudinal dependence described by a perturbation parameter δ . By solving the dispersion and transport equations for the local evanescent plane wave field, one may show that, to a lowest order in δ , the phase paths coincide with the contours of constant refractive index. Thus, the mode shape deforms and accommodates smoothly to the longitudinally-changing environment. This study is to be continued.

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SECTION II: SOLID STATE ELECTRONICS

A. X-ray Guided Wave Electronics

B. Post and H. J. Juretschke

1. Objectives

To use the anomalous propagation of x-rays in good crystals for developing guided-wave modes with optimal properties in thick crystals; to apply these modes to both the study of the solid state of the host crystal and the coupling of x-rays to other waves within the solid; and to examine coupled-mode techniques to determine their suitability for refining structure determination in crystallography.

Dynamical interactions of multiple x-rays within nearly perfect crystals are intended to lead eventually to special waveguides and components that can form the basis for possible future coherent x-ray circuitry. A second portion of the program involves the coupling of x-rays to other wave types, such as optical or acoustic waves, within the crystal. If the interactions prove to be sufficiently strong, these other waves can be used to modulate the x-ray beam, or to switch it from one state to another. Thus, the x-ray beam could be controlled electronically; otherwise, it would be necessary to turn the crystal mechanically to achieve the desired changes. The proposed program on x-rays thus involves a number of fundamental investigations which could make possible a systematic approach to x-ray circuitry.

2. Approach

Based on the dynamical theory of n-beam interactions of x-rays in crystals, and on the availability of good single crystals of ever increasing variety, we will carry out a combined program of theoretical exploration and experimental realization of the behavior of x-ray modes travelling along directions close to those specifying two or more Bragg conditions within the crystal. Since strong dynamical effects occur only within minutes of arc or less of these directions, the experimental methods require high spatial and energy resolution. Coupling to other types of waves will employ the general techniques of nonlinear optics already well-developed in other frequency domains.

3. Progress

- (a) A more detailed analysis of the three-beam case, in a form which allows ready generalization to four- and six-beam cases, has been carried out.¹ At the same time, we have attempted to extract from the general formulation a simple conceptual scheme that allows good qualitative predictions without having to repeat the whole analysis in each case. The results permit, among other effects, a strong optimization of x-ray transmission at the exact n-beam point with respect to the polarization of the incident beam. They also give a direct description of the shift of the polarization of the various modes as the direct beam passes through the n-beam point. Intuitive ideas about propagation efficiency as related to the structure of the real part of the dispersion surface have been formulated and are being tested. A number of experimental verifications of the fine

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structure of the interactions predicted by the theory have been postponed because of the imminent installation of a new 12.5 kW high intensity x-ray unit funded largely by JSEP through a special equipment appropriation.

- (b) In the experimental determination of the real part of the x-ray index of refraction by x-ray interferometric techniques, we have been able to improve existing approaches by the simple expedient of rotating a flat plate specimen in the x-ray beam within the interferometer. This avoids the difficulty inherent in the preparation of the commonly used wedges to achieve a continuously variable thickness. The new method for determining x-ray indices of refraction in an x-ray interferometer has been developed further,^{2,3} and has been aided by the installation of a better interferometer. This method is being applied to a number of materials as a promising procedure for routine determination of x-ray indices of refraction. The method is also being tested for applicability to synchrotron radiation where the full spectrum of wave lengths will be available. The study of two-beam interactions in a sample placed within the interferometer is being assembled.
- (c) The analysis of the two beam x-ray interaction with other waves, in the framework of dynamical theory, has led to the conclusion⁴ that such coupling is particularly effective in those geometries in which x-rays are close to total reflection from the crystal surface. For such Bragg reflections, involving surface mode-like x-ray modes within the crystal, phase matching can always be achieved for some direction of propagation of the other wave in the crystal, and the boundary conditions for the modified x-ray can easily be satisfied by superposition of the natural x-ray modes within the solid. This study has required extending of the traditional dynamical treatment of the dispersion surface into the regions of total reflection, and, in particular, towards utilizing the normally-forbidden modes with negative absorption coefficients. Such modes are permitted in this problem, because the source of the modified x-rays is really within the crystal. This approach has been applied to analyze an experiment⁵ that has had only cursory interpretations so far in order to test whether it can account for some of the unexplained quantitative asymmetries in line intensities and line shapes that are observed. Apart from reproducing the major features of the experiment, the theory also predicts some fine structure that thus far has not been seen and is probably obscured by the beam spread due to the experimental conditions which have not been completely specified. In an extension of this type of experiment, the theory also seems to predict some differences in thermal diffuse broadening of x-ray lines for reflected and transmitted diffracted beams, again probably only observable under stricter control of experimental parameters than is characteristic of typical x-ray experimentation.

The same theoretical approach has been applied to determine the optimum arrangement for the coupling of photons to x-rays in the symmetric Bragg geometry. It is expected that shifts in Bragg

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angle of the order of 200 seconds of arc are realizable for 6000 \AA light. Such a shift is easily observable, and should make possible the detection of rather weak x-ray-photon coupling. The experiment to look for this effect will be running shortly.

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B. Interaction of Millimeter Waves and Semiconductors

B. Senitzky

1. Objectives

The broad objective of this study is to investigate the interaction of millimeter wavelength radiation with mobile charge carriers in semiconductors. Although considerable work has been performed in this area at microwave frequencies,¹ far fewer investigations have been conducted at millimeter wavelengths.

The effect of conduction carriers on guided energy is characterized by a complex dielectric constant, which, in an appropriate structure, attenuates and/or changes the phase of the guided radiation. This principle is the basis for the familiar class of devices which includes modulators, phase shifters and switches.

When lumped semiconductor devices are used to control electromagnetic energy at microwave frequencies, the guiding structure must be designed so that radiation can interact effectively with the device. In other words, the structure must be matched to the device. At millimeter wavelengths, the matching structures become lossy, and factors such as junction capacity, lead impedance and device encapsulation further degrade the performance of the lumped device. On the other hand, at these frequencies, the electromagnetic structure becomes smaller and begins to approach the dimensions of the semiconducting device. The possibility, therefore arises, of matching the device to the structure rather than the other way around.

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One of our specific objectives is to study the feasibility of matching a P^+-I-N^+ diode to an electromagnetic structure to achieve extended interaction with 107 GHz radiation. Some qualitative work on the problem has been performed in the Netherlands² and in the Soviet Union³ in this frequency range. In contrast to the microwave frequency range, where the active region of the semiconductor is small compared to a wavelength, at millimeter wavelengths we must study a structure for which the active region is comparable to a wavelength. Such factors as the mobile charge density variation will now play a more significant role. We will use millimeter wave radiation to probe the active "intrinsic" region when known concentrations of mobile charge carriers are present due to the background impurity level. The results should yield some indication of the reliability of our measurement technique. We will then probe the intrinsic region when charge is injected from the contacts. Although there have been several theoretical predictions⁴⁻⁶ of the injected charge distribution, little or no experimental work has been performed on this subject. A better understanding of these and other related questions is required as a basis for the design of extended interaction semiconductor devices of millimeter wavelengths.

An important subsidiary objective is to determine under what operating conditions the injected carriers will change primarily the phase of the guided millimeter wave energy, and introduce minimal attenuation. Such performance would have significant device implications.

We will first study the interaction of 107 GHz radiation with a silicon P^+-I-N^+ diode in rectangular metallic waveguide and subsequently in silicon dielectric waveguide. The feasibility of fabricating the diode directly on the dielectric waveguide in order to achieve an integrated circuit with an active component, as discussed by H. Jacobs et al.,⁷ will be investigated.

2. Approach

The interaction of millimeter wave energy and mobile charge carriers in semiconductors will first be studied in a well-defined electromagnetic structure consisting of the dielectric slab-loaded, rectangular waveguide shown in Fig. 1. The slab consists of a silicon P^+-I-N^+ diode, oriented in the E plane of the guide. The guiding structure will be designed so that only the dominant mode, similar to the TE_{10} mode in air-filled guide,^{8,9} will be excited.

The slab thickness, t , and length, l , will be varied. If required, the slab height, b , can be decreased by using reduced height waveguide. At low charge concentration the interaction with radiation can be computed using perturbation theory.⁹ At higher charge concentrations the interaction can be computed directly from the boundary conditions. One of the advantages of the structure shown in Fig. 1 is that, even for relatively thin slabs (5 mils), the field in the dominant mode tends to concentrate in the slab and exponentially decay in the x direction so that the sensitivity of the interaction is enhanced.

We will measure the reflection and transmission properties of the structure and determine the complex dielectric constant from these measurements. A normal or reduced height slotted waveguide can be used to determine the charge distribution in the y (vertical) direction, and reflections in the absence of charge injection can be eliminated by tapering the silicon slab in the z direction.

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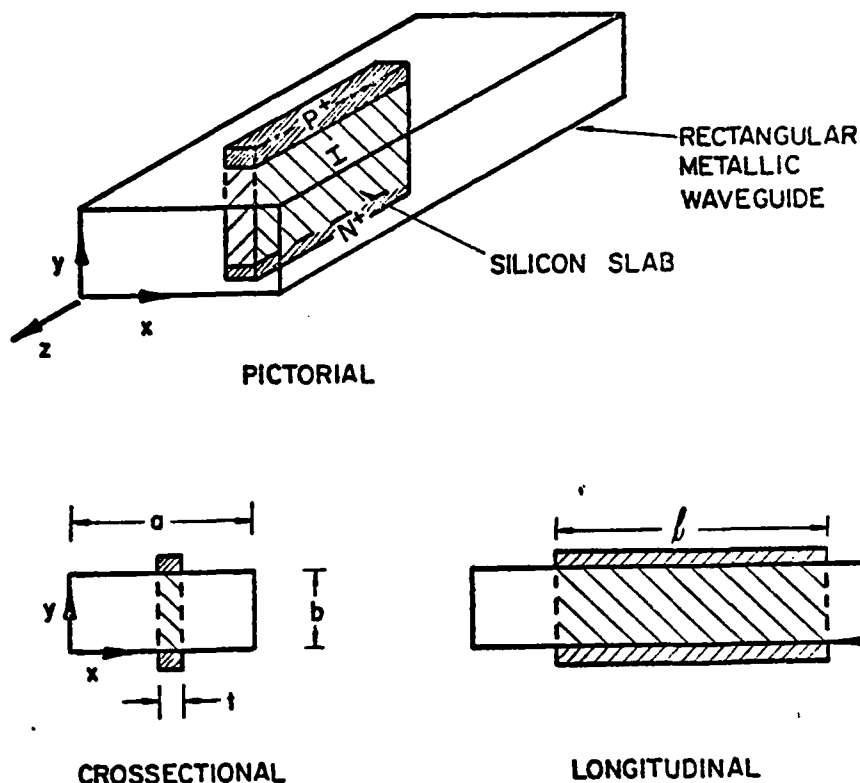


Fig. 1. P^+-I-N^+ diode in waveguide.

3. Progress

The circuit for transmission and reflection measurements at 107 GHz described in the Renewal Proposal dated 30 September 1978 has been assembled. The source is an extended-interaction oscillator with a rated power output of several watts. A precision attenuator, directional couplers, a ferrite switch, diode detectors and a wavemeter have been obtained and incorporated in the circuit. A diode mount consisting of a split copper block has been fabricated according to plan.

In order to test the mm-wave system and diode mount, transmission measurements were first performed on uniformly doped slabs of 50 ohm-cm and 20,000 ohm-cm material. The ratio of the incident power to the transmitted power T , was measured and was found to be in rough agreement with theory,⁹ as indicated in Table I.

Our next goal was to construct the P^+-I-N^+ diode. This diode must be such as to permit extended interaction with the incident millimeter wave radiation. Its electron-hole recombination lifetime must therefore be sufficiently long, and to insure this essential property the diode has to be specially fabricated.

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TABLE I. Transmission coefficient of uniformly doped slab.

Resistivity (Ω -cm)		T (dB)
50	Experimental	7.5
	Theoretical	6.9
20,000	Experimental	1.6
	Theoretical	0.5

Most of the effort in this study so far has been devoted to experiments related to determining an appropriate fabrication procedure. These experiments have shown that a diode with the required property can indeed be successfully fabricated. The fabrication steps are outlined in Fig. 2. The reason for using ion implantation and laser annealing in steps 1 and 2, rather than the more conventional techniques of thermal diffusion and thermal annealing, will now be discussed.

Carriers injected at the P^+ and N^+ contacts diffuse and drift towards the center at the intrinsic region. In order that the charge concentration remain uniform in the y direction (see Fig. 1), a long electron-hole recombination lifetime is required. Since thermal processing can introduce both chemical and physical crystal defects which act as recombination centers, the recombination lifetime must be monitored. We achieved this by illuminating the silicon wafer with light from a $5 \mu\text{sec}$ pulsed xenon flash lamp which was transmitted through a one-millimeter-thick silicon filter,¹⁰ and by measuring the decay of the conductivity. (With this technique the measured lifetime depends primarily on the bulk recombination rate and to a lesser extent on the surface recombination rate.)

We first diffused phosphorous and boron into a 600 ohm-cm, $300 \mu\text{sec}$ lifetime silicon wafer at 1100°C . The lifetime dropped to less than $5 \mu\text{sec}$, which is too low for our purpose. We then implanted the same elements using an ion accelerator¹¹ and thermally annealed the radiation damage at 750°C . Although this was the lowest temperature at which effective annealing, as indicated by resistivity measurements, took place, the recombination lifetime again dropped to too low a value. We then replaced the thermal annealing process by a laser annealing process.¹² In this technique, $0.53 \mu\text{sec}$ pulsed-laser radiation melts the silicon surface to a depth of one micron but leaves the bulk properties unaltered. Oscilloscope traces show dramatically the improvement in the lifetimes due to laser annealing.

The results of our experimentation to date indicate that a fabrication technique such as that outlined in Fig. 2 can keep the recombination lifetime of our P^+ -I- N^+ diode sufficiently high so that we might expect to achieve an appreciable extended interaction with millimeter wave radiation. We next expect to study these interactions.

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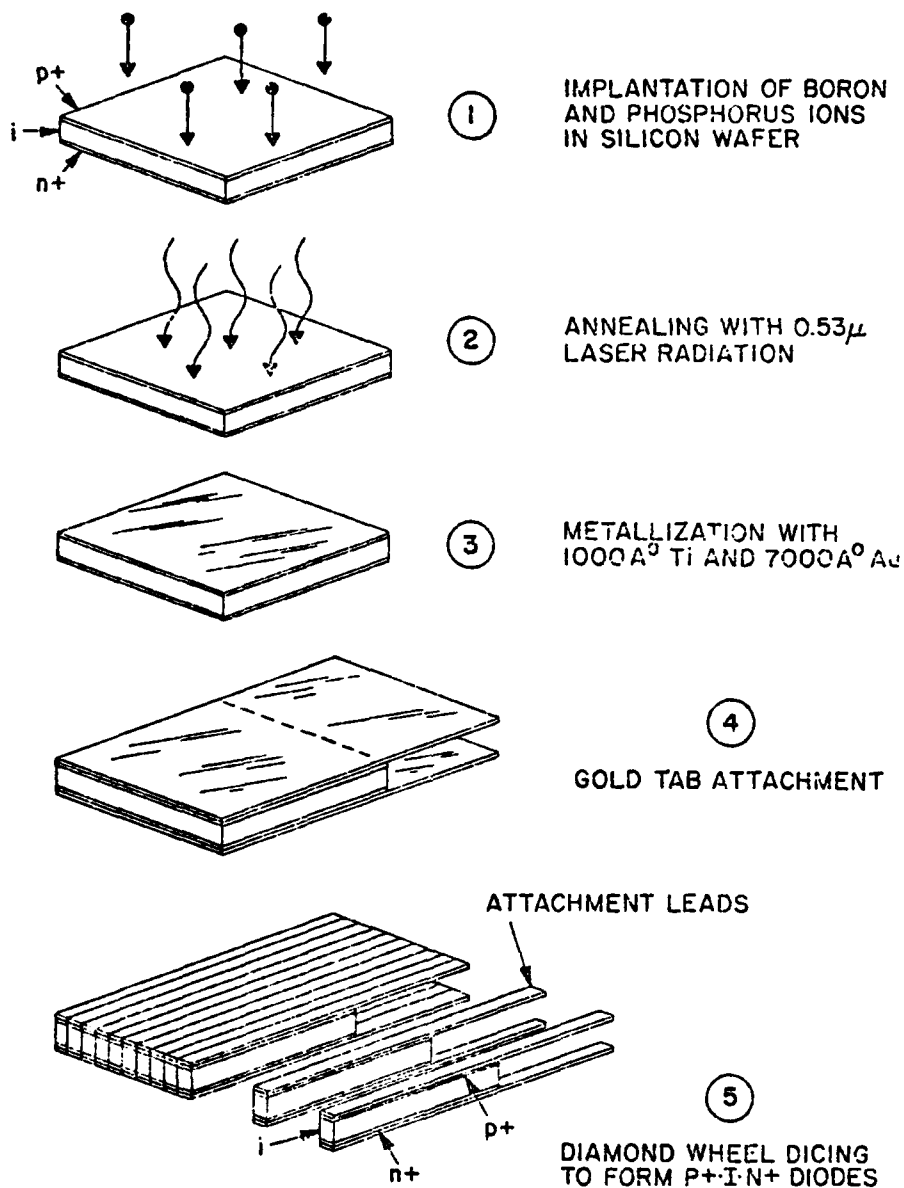


Fig. 2. Diode fabrication steps.

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C. Acoustoelectric and Acoustooptic Devices

W-C. Wang and H. Schachter

1. Objectives

The objectives are (a) to study the physical phenomena underlying the performance of surface acoustic wave devices employing nonlinear effects in semiconductors, and in the process to improve device performance or invent new devices. This includes: i) a study to increase the correlation efficiency using a BGO-Si-LiNbO₃ (BGO=Bi₁₂GeO₂₀) structure both for real-time and storage systems; ii) a novel acoustoelectric FM and AM demodulator; (b) to examine a new method for diagnosing the surface and interfacial conditions of a thin-film semiconductor by acoustoelectric means; (c) to study basic processes leading to efficient acoustooptical real-time and storage correlators.

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2. Approach

- (a) (i) The structures for the acoustoelectric correlator consist of a thin Si wafer ($\approx 10 \mu\text{m}$) inserted between two substrates, one of BGO and the other of LiNbO_3 . The Si wafer can either be a high resistivity Si (both p and n type, 10 to $100 \Omega\text{-cm}$) or a diode mosaic. The plain Si wafer is used to perform the function of real-time correlation and the diode mosaic is used to perform the function of correlation with memory.¹⁻³
- (ii) A new type of FM demodulator has been developed based on the strong space charge nonlinearity induced by SAW's in an adjacent semiconductor and on the filtering action generated by spatial integration over the length of the nonlinear interaction. This type of FM demodulator is structurally very simple and can be operated at high carrier frequencies; its performance is presently under study.⁴
- (b) A theory based on the nonlinear interaction between induced charges and fields has been developed in order to describe the operation of a semiconductor thin-film convolver at flat band. In the past, various convolver theories have been proposed and presented, but those theories were valid only for semiconductors of thickness large in comparison with the acoustic wavelength. One of the reasons for developing such a thin-film theory is that it will help in the diagnoses of thin-film surfaces and interfacial properties. Using SAW as a diagnostic tool, the advantages are (1) the depth of electric field penetration can be controlled by varying the sonic frequency; thus, the interfacial properties of the thin film can be investigated, (2) the diagnostic process is contactless and nondestructive, and (3) the electric field associated with the SAW's has both tangential and normal components, so that some of the thin-film orientational properties can be revealed. Computer results for thin-film convolvers at flat band have been obtained. Theories and models for the non-flat band case will be developed. The results will be used to evaluate the experimental outcomes.
- (c) The aforementioned acoustoelectric signal processors (correlators and convolvers, real-time and storage types) have their acousto-optical counterparts. The basic operational concepts are similar to those of the acoustoelectric type. The key success for an efficient acousto-optical device relies on the strength of the acousto-optic interaction. In this connection, we have found through a theoretical analysis of Bragg interaction of optically guided light and leaky surface waves⁵ that, for TM optical modes, X-propagating leaky waves on metallized 64° rotated Y-cut LiNbO_3 interact nearly twice as strongly at the surface as the free surface Rayleigh waves; thus, the 64° rotated Y-cut leaky surface wave offers the strongest acousto-optic interaction known to date. We intend to verify this experimentally.

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3. Progress

(a) Real-time and Storage Correlators

i) The study of the layered real-time correlator has been continued. As described previously, the structure consists of a very thin Si wafer sandwiched between two piezoelectric substrates. Using computational methods, we determined the correlation strengths as a function of thickness and frequency. The results are reported in a recent publication.⁶ The above study was done assuming a flat-band condition.

Next, we extended our study to non-flat band conditions. This state could exist either because of external sources or due to imperfections at the surface of the semiconductor. A study which could relate the output correlation voltage to the existence and strength of these surface states is of high interest. We determine the dc relations between outside sources or surface imperfections modeled as surface charges and the charge distribution inside a thin film semiconductor. Computational curves representing these relations are in the process of completion. We expect to continue this study by calculating the output correlation voltage as a function of the thickness and surface states and by comparing these results with the results from the thin film flat-band case to derive a diagnostic tool for detecting surface state charges.

ii) We continued our efforts to build a realistic model of the storage correlator. In a previous report, we mentioned that the diode mosaic was represented by two time-varying parts, a source and a load. The model was modified such that the source was considered to consist of an ac potential across the diodes, and a variable surface charge in the space between diodes. Both the ac potential and the surface charge were found by considering the diode mosaic as a load on the surface acoustic wave. Calculations to find the magnitude of the ac potential and the variable surface charge as a function of the input signal magnitude and frequency, taking into account the loading effects of the diode wave, were performed and results compared with experiments.⁷ Further refinements which take into consideration the thickness of the diode mosaic as well as variable geometries and conductivities are in process. This information should help in the design of an optimum storage correlator with respect to both geometry and frequency range.

(b) Acousto-Electric Demodulators

We continued our effort on using the acousto-electric correlator as a signal processor. In our previous report, we described its use as an FM demodulator at a carrier frequency of 100 MHz. By improving our experimental capability, we extended the range of this demodulator to 200 MHz with very good experimental results. Next, we developed a novel Differential Phase-Shifted Keyed (DPSK) demodulator. The DPSK input signal is applied simultaneously to two

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identical SAW transducers separated by a distance d such that d/v is equal to the bit interval T . The resulting two colinear surface acoustic waves are thus propagating in the same direction with a phase separation determined by T . The two waves pass under a semiconductor plate. The nonlinear interaction between induced electric fields and charges in the semiconductor followed by spatial integration across the semiconductor results in an output proportional to the phase modulation of the input signal. Theoretically, we found that one of the requirements for successful demodulation is that the bit interval T should be much larger than the equivalent integration time L/v where L is the length of the spatial integration. Experiments have been successfully carried out at a carrier frequency of 52 MHz, a bit interval of $13 \mu\text{sec}$ and an integration time of $1 \mu\text{sec}$. Experiments to extend the frequency range and to determine the effect of the condition $L/v < d/v$ upon bandwidths and bit rate will continue.

Next, we used the DPSK device as a base-band demodulator associated with spread spectrum correlator. Particularly interesting is that it may be possible to perform both the decoding of the code sequence underlying the spread spectrum and the demodulation of the base-band in an integrated device, thus reducing the number of elements needed to a minimum (one). The results obtained so far are reported in Reference 8.

(c) Thin-Film Diagnostics

i) Experiment: Epitaxially-grown GaAs films of different surface doping and with different thicknesses have been obtained. The surface doping varies from $3.5 \times 10^{15}/\text{cm}^3$ to $5 \times 10^{18}/\text{cm}^3$ and the thickness of the spi-layer varies from $0.3 \mu\text{m}$ to $3 \mu\text{m}$. The substrate is semi-insulating GaAs. We have succeeded in forming ohmic contacts on GaAs films (using Au-Ge). Only the sample with low resistivity, $3 \times 10^5/\text{cm}^3$, produced significant magnitudes of the dc acousto-electric field and the convolver output. We are in the process of utilizing the dc acousto-electric field measurement at different rf frequencies to determine both the carrier mobility and the trapping dynamics of the thin film. Further, in the film acousto-electric measurement one can clearly separate the contribution of the normal field component from that of the tangential component associated with the travelling SAW. (The separation of the two components has been difficult to achieve in the case of thick semi-conductors; the reason is not clear at present.) This separation is quite important since the tangential component is due solely to the drift velocities of the carriers; thus, the trapping effect on the drift mobility can be accurately determined.

ii) Theory: Acousto-electric signal generation due to SAW's for the case of semi-infinite semiconductors have been analyzed even with the inclusion of surface states. However, in the thin film case, analytical analysis (including diffusion and drift) has yet to be done.⁶ In order to correlate and understand the experiments

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and trapping dynamics, both the film thickness and the trapping charge on both the film surfaces must be taken into consideration. We have formulated³ theory and we are in the process of computing the signal generation due to SAW for both flat band and non-flat band cases.

(d) Acousto-optic Signal Processor

Progress in this area has deviated from what we proposed. Instead of following the proposed program, we have realized that ultimate progress in acousto-optics will be hampered seriously until good thin films with appropriate properties can be made available. We also have learned of new procedures to produce films of improved quality, and have therefore embarked on a new systematic program for the creation of high-quality thin films. Success in that program would constitute an important contribution in its own right.

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SECTION II: SOLID STATE ELECTRONICS

D. Electric and Magnetic Interactions in Thin Films and Surface Regions of Solids

H.J. Juretschke

1. Objectives

To understand the equilibrium properties, the approach to equilibrium, and the response to applied fields and waves of the surface regions of selected solids, both conductors and insulators, and to develop new methods for their investigation.

2. Approach

The experimental approach concentrates on the change of properties of solids when the surface/volume ratio of their geometry becomes significant. Transport properties are examined for their size effects, and on the influence of specific parameters, such as electrostatic charging, changes of composition or of order, or mechanically induced surface strains, on these size effects. Emphasis is on those special interactions that lead to nonlinear responses or to resonances, and on the coupling between the electromagnetic and elastic fields in the surface region. The theory will emphasize use of the methods developed in recent years for the study of defects in solids for the investigation of the surface, considered as an extended defect.

3. Progress

The initial part of the three-year program proposed in the Renewal Proposal dated 30 September 1978 is being implemented systematically. Although completed task results are not yet available, progress in most of the areas of the unit has been satisfactory, and according to schedule. Because of staff adjustments, the work on surface diffusion and microwave modelling has received less attention during this period, but will be activated shortly, although with less emphasis.

The program to determine the range of penetration of electrostatically-induced surface stresses is in full swing. A whole sequence of Au-Ag layers, a common total thickness but with different proportions of the two metals, is being tested. The Ag is at the mica interface, deposited epitaxially and annealed, and the Au is laid down subsequently, at room temperature, and without annealing, in order to minimize interdiffusion between the two layers. As the Ag thickness is reduced, we expect that surface stresses of the interface start to penetrate the Au layer, and will then show charge scattering characteristic of Au rather than Ag. On the other hand, the Maxwell stresses always penetrates the full sample thickness, and detect the presence of the Au overlay and its relative thickness at all stages of the experiment. Because the Au layer is not annealed, its resistivity is higher than that of bulk gold. As a consequence, size effects at the outer surface, which might complicate the analysis of the experiment, are minimized. At the same time, this increased resistivity leads to an increase in the signal level of the changes of surface resistance with charge, and is therefore detectable with greater accuracy. We also see some evidence in this signal of contributions of interlayer scattering by the conduction electrons at the Au-Ag interface.

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A long range experiment has been started to identify the cause of the aging effects observed in the stresses at the mica-Cu interface. We suspect that oxygen diffusion through grain boundaries in the copper film is responsible for slow oxidation of this interface. As a test of this hypothesis, simultaneously-prepared twin samples of copper are being monitored over an extended time period, with one kept under vacuum and the other remaining exposed to the atmosphere. As part of this program we have reactivated a measuring system for detecting very low signal levels through vacuum seals in the presence of strong driving fields.

The design and building of the apparatus for extending the temperature range over which surface stresses can be measured down to liquid helium temperatures is near completion. We will use the existing temperature gradient in a liquid helium storage dewar to hold the sample at an arbitrary temperature above 4°K. A new electronic detection system has been built, with increased stability and reduced noise, and the sample holder for the metal-air-metal configuration has been assembled. In the near future, the system will be tested at liquid N₂ temperature before the final details of the hookup to the helium bath are arranged.

In the area of thin-line Metal-metal Oxide-Metal (MOM) junctions, we have been able to develop the proper fabrication parameters to produce junctions which, at room temperature, have rather high resistance and have pronounced nonlinear I-V behavior, characteristic of tunneling, at quite low currents. Since the method of fabrication closely simulates the effects that might take place at naturally-oxidizing grain boundaries or microscopic cracks at metal surfaces, our results suggest that nonlinearities of the type we observe are a natural feature of commonly-weathered metal surfaces, and must be taken into account when dealing with the electrical response of such surfaces. Our evidence indicates that part of the resistance ascribed to the junction is probably contributed by the continuously-decreasing width of the sample portion that remains metallic after oxidation, and also that the junction width itself, limited by how thick the metallic layer can be oxidized, is varying along the thickness of the junction. Both factors require a more careful analysis of the experimental data than is applied to the usual parallel-face very-thin-oxide configuration.

The experiment has been set-up to search for the surface strain-induced generation of second harmonic light in the reflected light at metal surfaces. The strains are produced by electrostatic charging. We look for this interaction in the walls of an optical waveguide where the light undergoes 100 or more reflections, with the two mirror surfaces chosen such that each reflection reinforces the conversion. This is expected to occur when a surface charge has oppositely-directed effect on the surface strains of the two mirrors. The final choice of wall materials will await preliminary investigation of the strains at metal-quartz interfaces, which are not known at present. Fused quartz was chosen as the waveguide medium in order to permit transmission of the ultraviolet generated by the harmonic conversion of red light.

In the area of surface magnetism, a model based on a generalized mean-field approximation has been applied to surfaces, and found to reproduce the Landau-Ginzburg relations, as well as to incorporate a new nonlinear term important at low temperature. We have found a method of solving the nonlinear equations exactly. Furthermore, methods have been developed for efficiently

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solving the perturbation of the spin wave spectrum in the Heisenberg model when the exchange interaction of surface spins differs from the bulk value. This can be done in analytic form, and allows a direct evaluation of spin wave phase shifts and surface magnetization.

E. New Solid State Materials

E. Banks

1. Objectives

To synthesize, characterize and measure the physical properties of new solid state materials. Such materials are potentially ferroelectric (and optically nonlinear), ferromagnetic, fluorescent or semiconducting, all of which have considerable technical interest and value if the properties investigated can be applied to practical devices. Even when they are not of immediate practical value, the study of their properties can lead to understanding that may point the way to the design of improved materials.

2. Approach

Attempts to synthesize new materials with interesting electronic properties are based either on modifying existing materials (e.g., by forming solid solutions) or by attempting the synthesis of materials based on theories which attempt to explain the dependence of the relevant property, e.g., ferromagnetism, on features of crystal structure and chemical bonding. New materials are characterized by crystallographic methods and measurement of relevant electronic properties such as optical spectroscopy, fluorescence, magnetic properties, Mossbauer spectra, conductivity and dielectric properties.

3. Progress

(a) New Fluorescent Mixed Fluorides of Divalent Rare Earths

Most of our current effort is devoted to attempts to grow single crystals of SrMgF_4 as a model for EuMgF_4 and SrMgF_4 and as the basis for studies of structure and metal-metal interactions in dilute systems. Some indications of possible success were found in Bridgman pulling of melts containing excess MgF_2 , compared to the stoichiometric composition. Single crystal regions of SrMgF_4 were observed. Structure factor calculations on EuMgF_4 , using a centrosymmetric space group, have led to improved agreement with observed X-ray intensities, compared to the non-centrosymmetric model based on the BaMnF_4 structure. Fluorescence lifetime measurements of the $\text{Eu}_{1-x}\text{Sm}_x\text{MgF}_4$ system indicate significant shortening of the lifetime of the Eu^{2+} emission with addition of Sm^{2+} , going from about 10^{-6} sec in EuMgF_4 ($x=0$) to about 10^{-7} sec in $\text{Eu}_{0.99}\text{Sm}_{0.01}\text{MgF}_4$, indicating that the energy transfer from Eu^{2+} to Sm^{2+} is largely non-radiative.

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(b) Proposed New Ferromagnetic Oxides

It was proposed that perovskite-type compounds containing ordered Mn^{4+} and Fe^{3+} would be ferromagnetic if the ions were well ordered. The ordering by charge difference was to be enhanced by using large divalent ions in the A sites of the ABO_3 type, with small trivalent ions. An attempt to prepare $\text{Ba}_{0.5}\text{Y}_{0.5}\text{Mn}_{0.5}\text{Fe}_{0.5}\text{O}_3$ led to the formation of two separate phases, BaMnO_3 and YFeO_3 . When Gd^{3+} (somewhat larger than Y^{3+}) was used, a single phase of perovskite type was formed. It is not ferromagnetic at room temperature, but no measurements have been made at lower temperatures. We are now attempting to use density measurements and chemical analysis to determine whether the iron and manganese are in the desired valence states.

F. Electronic Properties of Hydrogen in Solids

D. C. Mattis

1. Objectives

To develop first principles and theoretical techniques for relating the observed behavior of the hydrides of transition and rare earth metals and their alloys to their underlying electronic properties. The mathematics will be applied to the bulk, surface and transport properties of these materials. A study of the broader question of the electronic properties of hydrogen in metals will be conducted.

2. Approach

The behavior of hydrogen in solids is fast becoming one of the most important and unsolved problems of modern science. Despite astronomical efforts resulting in a vast body of mostly empirical knowledge,¹ little has been achieved in the nature of a comprehensive theory or an understanding that can be used for predictions. Currently, interest in the study of the electronic properties of hydrogenated solids is increasing, especially because of the existence of major unsolved problems whose resolution bears on the use of solids in electronic energy conversion and transmission. On a fundamental level, the electronic structure of defects lies at the forefront of current theoretical interest. Substitutional or interstitial hydrogen is one of the simplest possible solid-state defects, a near ideal testing ground for theories of impurities in solids. Its simple electronic structure also accounts for the many studies of its interaction with surfaces, catalysis and chemisorption. Recent theoretical work has laid the groundwork for attacking many of the important roles of hydrogen in solids from a fundamental point of view.

The combination of the approach of J. Friedel and co-workers,² relating the observed behavior of transition metals to many-body effects, and methods developed by us³ for studying the response of interacting particles to various defects, will form the foundation for a theory of hydrogen in transition and rare-earth metals that has direct applicability to the many and startling effects

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observed in these systems. Ground state properties of the unperturbed metal system will be described by a variational Cutwiller-type wave function,⁴ and schemes will be developed for applying modern techniques to the study of its excitation spectrum. The effect of hydrogen impurities is then treated by many-body perturbation theory of both the ground state and its excitations, in order to permit the description of time-independent and time-varying properties of the solids resulting from the presence of hydrogen impurities.

3. Progress

Our initial studies have resulted in the discovery of a new boson procedure Self-consistent Late Bosons (SLB) for the treatment of the electronic properties of impurities in metals and alloys. This procedure differs from our previous boson method in that the SLB bosons are renormalized in a self-consistent manner which incorporates the mean-field properties of fermi surface electrons. This represents an important discovery. Its application to the simplest metallic impurity problem, the Wolff model, reveals an entire realm of new physics and yields results which are qualitatively different from those of our earlier boson procedure.⁵

In addition, the SLB method permits a natural accommodation of Friedel's sum rule.⁶ We are now able to study the role of screening by conduction electrons in determining the observed properties of hydrogen in metals and alloys. Also, we are able to examine the role of electron correlation in the neighborhood of the hydrogen impurity and may, therefore, explicitly analyze the difference between the interaction of hydrogen with s-electrons as opposed to that with d-electrons, including the role of band degeneracy.⁷ The importance of these developments lies in the fact that hydrogen is known to interact strongly with metallic systems which are rich in d-electrons, and weakly with those in which d-electrons are absent. We may now completely characterize the local, conduction electron environment in both cases.

Presently we have completed an SLB diagonalization of the Hamiltonian for a hydrogen impurity in an s/d-band metal. Two questions are currently under study:

- (a) The effect hydrogen has on the superconducting properties of the metal, i.e., hydrogen in palladium. Preliminary results are available; however, further analysis is required.
- (b) Nuclear Magnetic Resonance (NMR) is a powerful and sensitive experimental technique for the characterization of the local electronic environment of the hydrogen impurity.⁸ The SLB method predicts the existence of a new mass-isotope effect in the Knight Shift of the NMR line. This effect is predicted to be sensitive to conduction-electron screening of the hydrogen (or positive muon) impurity. Calculations are being carried out.

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SECTION III: INFORMATION ELECTRONICS

A. Reduced Order Models of Large Scale Systems

D. C. Youla, F. Kozin and J. J. Bongiorno, Jr.

1. Objective

Our objective is to produce reduced-order models for large-scale systems by a combination of time-domain, statistical and aggregation-like methods. The objectives can be divided into two major efforts:

- (1) Study and develop useful computationally stable and efficient order reduction techniques. These techniques must yield good approximations of the dynamical quantities to be monitored.
- (2) Study and assess the effectiveness of reduced order model control designs when applied to the original large scale system.

2. Approach

Society is comprised of a multitude of large scale systems. Communications, transportation, power, defense, waste disposal, and agriculture are but a few of the system substructures upon which our society is based. The heavy demands put upon these large systems by a society that continues to develop, as well as the desire to keep the systems themselves developing and operating in some reasonably efficient, safe, and cost-effective fashion, of necessity, requires intensive monitoring of each of the systems. However, the magnitude of these systems makes in-detail monitoring prohibitively costly even with current high-speed high-capacity computers. Reduced order models, therefore, must be developed.

Problems to be studied for reduced order models include: On what basis shall we construct a reduce order model? What criteria shall be employed to arrive at a reduced-state model of the original system? What significant dynamical characteristics of large scale systems can be predicted from lower order models? Finally, how effective are design studies generated by lower order models when applied to the original large scale system? Parameters and state evolution may not be known exactly. Hence, there is uncertainty, either stochastic or deterministic, in our knowledge of the system. This fact must be accounted for in our development of order-reducing procedures, and their related computational algorithms. Thus, for example, the methods must be stable in the sense that small observation noise will not lead to large errors.

In our proposed research program, we shall be concerned with three major problem areas:

- (1) Analytical and computational methods for order reduction.
- (2) Applicability of control design concepts, generated from reduced order models to the original large scale system.
- (3) Implementation to real large scale systems.

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3. Progress

During the first year we have succeeded in obtaining a complete solution to the multichannel problem of spectrum recovery from a given finite set of (matrix) covariance samples. This result, in our opinion, has immense practical and far-reaching implications. In addition, further gains have been made in coupling together the notions of complexity and model identification in one quantitative statistical formulation. These results are presented in this section where we shall describe some of the concrete results obtained in the focal areas of spectral estimation, model fitting and reduced-order modeling by aggregation. Each of the three items (a) Youla, (b) Kozin, and (c) Bongiorno is preceded by a brief description of its intent and significance.

(a) Solution of the Multichannel Interpolatory Spectral Estimation Problem

Let \underline{x}_t denote a discrete-time m -dimensional random vector process where " t " can traverse all positive and negative integers. Let us also suppose that the process is zero-mean and second-order stationary. Then,

$$E(\underline{x}_t \underline{x}_{t+k}^*) = C(k) \quad , \quad |k| = 0 \rightarrow \infty \quad , \quad (1)$$

is the associated $m \times m$ covariance function.* Clearly, for all integers k ,

$$C(-k) = E(\underline{x}_t \underline{x}_{t-k}^*) = E(\underline{x}_{t+k} \underline{x}_t^*) = C^*(k) \quad . \quad (2)$$

As is well-known,¹ if the power spectrum $F(\theta)$ of the process is absolutely continuous, there exists an $m \times m$ hermitean nonnegative-definite spectral density matrix $K(\theta)$, whose entries are absolutely integrable over $-\pi \leq \theta \leq \pi$ and is such that,

$$C(k) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-jk\theta} K(\theta) d\theta \quad . \quad (3)$$

Hence,

$$K(\theta) = \sum_{k=-\infty}^{\infty} C(k) e^{jk\theta} \quad (4)$$

and the $m \times m$ covariance samples $C(k)$, $|k| = 0 \rightarrow \infty$, emerge as the Fourier coefficient of $K(\theta)$.

* Column-vectors are written \underline{a} , \underline{x} , etc., and if A is any matrix, \bar{A} is its complex-conjugate, A' its transpose, $A^* (= \bar{A}')$ its adjoint, $\det A$ its determinant, A^{-1} its inverse and $\text{Tr } A$ its trace. As usual, if $A = A^*$ is hermitean, $A \geq 0$ (> 0) means that A is non-negative-definite (positive-definite). In addition, I_m , $0_{m,k}$, $0_m (= 0_{m,m})$ and $\underline{0}_m$ denote the $m \times m$ identity, the $m \times k$ zero matrix, the $m \times m$ zero matrix and the m -dimensional zero vector, respectively. We also abbreviate "almost everywhere" by a.e. and "if and only if" by iff.

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A nondeterministic process x_t is one whose future is not perfectly predictable from its present and past. Such is the case iff $K(\theta)$ satisfies the Paley-Wiener finite-entropy criterion,*

$$\text{Entropy}(K) \equiv \frac{1}{2\pi} \int_{-\pi}^{\pi} \ln \det K(\theta) d\theta > -\infty. \quad (5)$$

It can be shown² that (5) implies the infinite set of inequalities,

$$T_k \equiv \begin{bmatrix} C(0) & C(1) & \dots & C(k) \\ C(-1) & C(0) & \dots & C(k-1) \\ \dots & \dots & \dots & \dots \\ C(-k) & C(-k+1) & \dots & C(0) \end{bmatrix} > 0, \quad k=0 \rightarrow \infty. \quad (6)$$

We are now in a position to explain the solution that we have obtained to the following very important practical problem: Given that the process x_t is non-deterministic and possesses an absolutely continuous spectral function, find an explicit parametric formula which generates the entire set of admissible spectral densities $K(\theta)$ whose first $n+1$ Fourier coefficients are the known, error-free, partial covariance data $C(0), C(1), \dots, C(n)$.

Solution. Let T_n and $T_n(-1)$ denote the block-Toeplitz matrices (6) constructed on $C(0), C(1), \dots, C(n)$ and on the "reversed" data $C(0), C(-1), \dots, C(-n)$, respectively. (Clearly, $T_n(-1)$ is the result of replacing each $C(k)$ in T_n by $C(-k)$, $k=1 \rightarrow n$.) Also, let

$$\bar{\xi}(z) = (1_m \quad z1_m \quad \dots \quad z^n 1_m)' \quad (7)$$

1) Effect the (unique) Gauss factorizations,

$$T_n = \Delta_n^* \Delta_n, \quad T_n(-1) = \Delta_n^*(-1) \Delta_n(-1) \quad (8)$$

where Δ_n and $\Delta_n(-1)$ are both lower-triangular with positive diagonal scalar entries. Let M_n and $M_n(-1)$ represent the two submatrices formed with the first m columns of Δ_n^{-1} and $\Delta_n^{-1}(-1)$, respectively.

2) Define two $m \times m$ polynomial matrices

$$P_n(z;1) = M_n^* \bar{\xi}(z), \quad (9)$$

$$P_n(z;-1) = \bar{\xi}'(z) M_n(-1) \quad (10)$$

*The inequality $\text{Entropy}(K) < +\infty$ is automatic.¹

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and let^{*}

$$D_n(z) \equiv P_n(z;1) - z \rho(z) \tilde{P}_n(z;-1) \quad (11)$$

- 3) Then, all admissible interpolatory solutions $K(\vartheta)$ are encompassed by the formula

$$K(\vartheta) = D_n^{-1}(e^{j\vartheta})(1_m - \rho(e^{j\vartheta})\rho^*(e^{j\vartheta}))D_n^{-1}(e^{j\vartheta})^* \quad (12)$$

where $\rho(z)$ is an arbitrary mxm bounded^{**} matrix function of z such that

$$\text{Entropy}(1_m - \rho\rho^*) > -\infty \quad (13)$$

Several explanatory comments are in order.

First, $\tilde{P}_n(z;1)$ and $\tilde{P}_n(z;-1)$ may be identified, respectively, with the standard left and right orthonormalized matrix polynomials of degree n associated with the moment sequence $C(0), C(1), \dots, C(n)$.²⁻⁴ This means that $P_n(z;1)$ and $P_n(z;-1)$ satisfy generalized recursions of the Levinson type and all the highly efficient software that has been developed for the multichannel maximum-entropy estimator (MEE)⁵ can be used intact to implement (12).

Second, the maximum-entropy estimator $K_{ME}(\vartheta)$ is the special case of (11) and (12) with $\rho(z)$ chosen equal to the identically zero matrix. Hence,

$$K_{ME}(\vartheta) = (P_n^*(e^{j\vartheta};1)P_n(e^{j\vartheta};1))^{-1} \quad (14)$$

a familiar expression.⁵

Third, it follows directly from (12) that

$$\text{Entropy}(K) = \text{Entropy}(K_{ME}) + \text{Entropy}(1_m - \rho\rho^*) \quad (15)$$

Since $\text{Entropy}(1_m - \rho\rho^*) \leq 0$ (because $\rho(z)$ is bounded),

$$\text{Entropy}(K) \leq \text{Entropy}(K_{ME}) \quad (16)$$

with equality iff $\rho(z) \equiv 0_m$ and $K(\vartheta) = K_{ME}(\vartheta)$.

Fourth, the basic relationship (15) and the formula

$$\text{Entropy}(1_m - \rho\rho^*) = -\frac{1}{2\pi} \int_{-\pi}^{\pi} \ln \det^{-1}(1_m - \rho(e^{j\vartheta})\rho^*(e^{j\vartheta}))d\vartheta \quad (17)$$

^{*} $\tilde{P}_n(z;-1) \equiv z^n P_n^*(1/\bar{z};1)$.

^{**} $\rho(z)$ is bounded if (a) it is analytic in $|z| < 1$, and (b) $1_m - \rho(z)\rho^*(z) \geq 0$, $|z| < 1$.

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suggest strongly that the quantity

$$\frac{1}{2\pi} \ln \det^{-1} (I_m - \rho(e^{j\hat{\theta}}) \rho^*(e^{j\hat{\theta}})) \quad (18)$$

deserves the name of entropy echo-loss density at angle $\hat{\theta}$. An FEE, or flat-echo estimator, is one for which this density is a constant.

One particularly simple and numerically effective way to generate FEE's is to choose

$$\rho(z) = \mu d(z) \quad (19)$$

where μ is an arbitrary constant mxm matrix such that

$$I_m - \mu \mu^* > 0, \quad (20)$$

and $d(z)$ is an arbitrary rational mxm regular all-pass.*

Thus, for this subset of FEE's,

$$K_{FE}(\hat{\theta}) = D_n^{-1}(e^{j\hat{\theta}}) (I_m - \mu \mu^*) D_n^{-1}(e^{j\hat{\theta}})^* \quad (21)$$

where

$$D_n(z) = P_n(z; 1) - z \mu d(z) \tilde{P}_n(z; -1) \quad (22)$$

Furthermore,

$$\text{Entropy}(K_{FE}) = \text{Entropy}(K_{ME}) - \ln \det^{-1} (I_m - \mu \mu^*) \quad (23)$$

Observe, that according to (23) it is possible to fix the entropy of $K_{FE}(\hat{\theta})$ in advance by a proper choice of μ and the all-pass $d(z)$ can then be designed with complete freedom to meet other engineering specifications. For example, it is possible to "tune" $K_{FE}(\hat{\theta})$ at one or several prescribed values of $\hat{\theta}$. Although this tuning procedure is well understood in the scalar case,⁶ much remains to be done for general m . Nevertheless, the prospects appear most promising and the entire matter is currently under careful investigation.

(b) Results on the Model Fitting Problem for Statistical Data

We have studied means by which observed data can be fit by one of a suitable chosen class of dynamical models. It is assumed that this class of models is described by some fundamental vector of parameters. This parameter vector

* $d(z)$ is a regular all-pass if (a) it is bounded (footnote ** on page 96) and (b) it is unitary on the boundary of the unit circle; i.e., $d(e^{j\hat{\theta}}) d^*(e^{j\hat{\theta}}) = I_m$. It is also rational if all its entries are rational functions of z .

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will include coefficient terms in the model as well as (for lack of a better phrase) a complexity parameter.

The complexity parameter is the dimension of the vector, which may be related to the order of a linear model or, perhaps, the highest nonlinear power term in the model.

It is assumed that the unknown parameters (components of the parameter vector) are to be estimated through some functional q of the N observed data values Y_N . We write

$$q_N(\hat{\theta}_K) \equiv q(Y_N; \hat{\theta}_K) \quad , \quad (24)$$

where $\hat{\theta}_K$ is the parameter vector to be estimated.⁷

For an assumed value K , the estimate $\hat{\theta}_K^N$ based upon the N observations is given by

$$\hat{\theta}_K^N \equiv \arg \min_{\theta_K} q_N(\theta_K) = q_N(\hat{\theta}_K^N) \quad . \quad (25)$$

Here it is assumed that $q_N(\theta_K)$ is a continuous function of θ_K on the compact domain Θ_K , that $q_N(\theta_K)$ has a unique minimum on Θ_K , and that for each K , we define $\hat{\theta}_K^N \in \Theta_K$ by

$$\arg \min_{\theta_K \in \Theta_K} \lim_{N \uparrow \infty} E \{ q_N(\theta_K) \} = \lim_{N \uparrow \infty} E \{ q_N(\hat{\theta}_K^N) \} \quad . \quad (26)$$

Under certain simple smoothness and uniform convergence conditions on $q_N(\hat{\theta}_K^N)$ as well as on its expectations we have been able to establish that the estimator $\hat{\theta}_K^N$, defined by

$$\arg \min_{1 \leq K \leq l} \arg \min_{\theta_K \in \Theta_K} q_N(\theta_K) = q_N(\hat{\theta}_K^N) \quad (27)$$

(where l is some arbitrary upper bound on K) satisfies

$$\lim_{N \uparrow \infty} \hat{\theta}_K^N \overset{o}{=} \theta_K^o \quad \text{with probability one}$$

where θ_K^o is the "true" parameter vector and K is its "true" dimension or complexity of the model. Finally, the limit

$$\lim_{N \uparrow \infty} \arg \min_{1 \leq K \leq l} E \{ q_N(\hat{\theta}_K^N) \} = Q(\hat{\theta}_K^o) \quad (28)$$

exists. This allows us to develop a general criterion leading to an estimate of the true complexity

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For "large" N , we can approximate $Q(\hat{\theta}_K^0)$ as

$$Q(\hat{\theta}_K^0) \approx \min_{1 \leq K \leq l} E\{q_N(\hat{\theta}_K^N)\} . \quad (29)$$

Under the smoothness and uniform convergence assumptions on q_N , along with the further assumption of asymptotic normality of the parameter vector $\hat{\theta}_K^N$, for each $1 \leq K \leq l$, we have the estimate

$$\min_{1 \leq K \leq l} E\{q_N(\hat{\theta}_K^N)\} \approx \min_{1 \leq K \leq l} \left[q_N(\hat{\theta}_K^N) + \frac{1}{2} \text{trace } H(\bar{\theta}_K) \Gamma(\bar{\theta}_K) \right] , \quad (30)$$

where $\bar{\theta}_K$ is defined above, Γ is the $K \times K$ covariance matrix of the asymptotic normal vector, and $K \times K$ matrix H is defined by

$$H = \lim_{N \uparrow \infty} (H_{ij}(N)) , \quad \text{where} \quad (31)$$

$$H_{ij}(N) = \frac{\partial^2}{\partial \hat{\theta}_K^i \partial \hat{\theta}_K^j} q_N(\hat{\theta}_K^N) .$$

Here, the result (30), in principle, allows us to determine an estimate of the "complexity" of a model from some prescribed class that fit the observed data. This estimate is obtained by calculating the terms in the brackets in (30) for each K and selecting that K that yields the minimum value. Notice that we have not put any specific requirements on the nature of the class of models or on the estimator q . Thus, it appears to us that a broad range of model fitting problems can be treated in which the q function estimator is naturally determined by the nature of the chosen models.

It is interesting to note that if q is the log likelihood function

$$q_N(\hat{\theta}_K) = -\frac{1}{N} \log p(Y_N | \hat{\theta}_K) , \quad (32)$$

and if q_N is quadratic in the component of the vector $\hat{\theta}_K$, then it can be shown that

$$H^{-1}(\bar{\theta}_K) = \Gamma(\bar{\theta}_K) \quad \text{for each } K .$$

Here the trace term in (30) becomes

$$\frac{1}{N} \text{trace } H(\bar{\theta}_K) \Gamma(\bar{\theta}_K) = \frac{1}{N} \text{trace } I_{K \times K} = \frac{K}{N} . \quad (33)$$

If (32) and (33) are placed in (30), one simply obtains the so-called AKAIKE Information Criterion (AIC)

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$$\min_{1 \leq K \leq \ell} \left\{ -\frac{1}{N} \log p(Y_N | \hat{\theta}_K^N) + \frac{K}{N} \right\} . \quad (34)$$

The result (30) becomes a natural generalization to the AIC procedure (34) for broader classes of models.

The applicability of (30) to various linear and nonlinear models will be studied in connection with part B - Statistical Techniques for Order Reduction - of this section. Furthermore, the connection between this statistical method and deterministic identification schemes such as Prony's method will be investigated.

(c) Control Design Concepts from Reduced Order Models

The main purpose of reduced order models is to reduce the cost of monitoring large scale systems. There is, however, one further potentially significant application of reduced order models, that is, their application to design of controllers for the original large scale system. In this connection, the approach of modeling large scale systems by lower order "aggregate" models appears to hold promise.

This idea of aggregation was first introduced by Aoki. The basic concept is as follows: Given an n -dimensional time-invariant dynamical system

$$\dot{x} = Ax + Bu \quad (35)$$

there exists an m -dimensional time-invariant dynamic system, $m < n$, given by

$$\dot{z} = Fx + Gu \quad (36)$$

for which

$$z(t) = Cx(t), \quad \forall t \geq t_0 \quad (37)$$

provided one can find a matrix F satisfying

$$FC = CA \quad (38)$$

and provided

$$G = CB \quad (39)$$

$$z(t_0) = Cx(t_0). \quad (40)$$

When (40) is not satisfied, it is easy to show that the error

$$e(t) = z(t) - Cx(t) \quad (41)$$

satisfies

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$$\dot{e} = Fe \quad (42)$$

Any matrix C for which (38) admits a solution for F is called an aggregate matrix for (35) and (36) is an aggregate system model. Clearly, the identification of the class of all aggregate matrices C in a way that permits an "optimal" one to be selected is highly desirable. Suppose for example that

$$y = Hx \quad (43)$$

is the output associated with the state equation (35) where H is not an aggregate matrix. Then $z(t) \equiv y(t)$ is generally not possible, but one might consider choosing an optimal C so that

$$J = \int_0^{\infty} (z-y)' Q (z-y) dt \quad (44)$$

is minimized, where Q is some selected symmetric non-negative definite or positive definite matrix. Many other possibilities can be conceived, and research along these lines is wide open.

Of particular importance is the optimal choice of C with respect to a performance measure which has practical operational significance. Specifically, one is not so much concerned with modeling (35) and (43) accurately, but rather in obtaining a lower order model which can be used successfully to find practical feedback control schemes or hierarchical control policies for the original system. Hence, the choice of C should be optimized with respect to a performance index which measures or adequately reflects the intended objectives. The evolution of satisfactory solutions to this important problem constitutes a long-range research program which must consider approaches in both the time domain and the frequency domain. At all stages, the fact that the difficulties with large scale systems are primarily computational ones must be constantly kept in the foreground of the research endeavors. In the following paragraphs, we describe some results already obtained which we believe contain some original observations, and which we hope will clarify the above points. Attention is restricted to those cases for which $H=C$ is an aggregate matrix.

Consider the possibility of employing the aggregate system model to determine a stabilizing control law for the original system. We have established:

Lemma 1. The output feedback control law

$$u = Ky = KCx \quad (45)$$

($H=C$ an aggregate matrix is assumed) in which K is any constant real matrix which stabilizes the controlled aggregate system model (i.e., ensures that the real part of every eigenvalue of $F+GK$ is negative), stabilizes the original system if, and only if, every eigenvector of A in the null space of C has an associated eigenvalue whose real part is negative.

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This lemma is a consequence of the fact for any aggregate system model that every eigenvalue of $F+GK$ is an eigenvalue of $A+BKC$, and any eigenvalue of $A+BKC$ which is not an eigenvalue of $F+GK$ has an associated eigenvector v in the null space of $C(Cv=0)$. Hence, the only eigenvalues of $A+BKC$ which are not eigenvalues of $F+GK$ are the eigenvalues of A associated with the hidden or observable system modes. One can show that these modes are always present whenever (38) is satisfied, and $m < n$. Clearly, whenever freedom exists in the choice of C , this matrix should be selected so that the associated hidden modes of A are asymptotically stable. No provision to assure that this is the case is made in a recently proposed algorithm⁹ for generating an aggregate system model. This algorithm leads to an aggregate system model in which the hidden modes are those associated with the eigenvalues of A which are large in magnitude. In view of Lemma 1, however, the aggregate system model obtained in this way will be quite useless unless these hidden modes are asymptotically stable. This of course is guaranteed when all the eigenvalues of A have real parts that are negative. We are presently considering an approach which avoids difficulties of this type and allows us to treat cases in which the original system can be unstable.

Instead of simply selecting the matrix K in (45) to stabilize the system, one might instead consider an optimal choice. In the well-known infinite-time output regulator problem this would call for the choice of K which minimizes

$$J = \int_0^{\infty} (y'Qy + u'Ru)dt, \quad (46)$$

where Q is a symmetric non-negative definite matrix and R is a symmetric positive definite matrix. We have established that when $H=C$ is again an aggregate matrix, the choice

$$K = -R^{-1}G'M \quad (47)$$

is optimal where M is the symmetric positive definite solution of the algebraic Riccati equation (controllability of the aggregate system is assumed)

$$F'M + MF + Q - MSM = 0 \quad (48)$$

and

$$S = GR^{-1}G'$$

Now, it is easily shown that the eigenvalues of $F+GK$ all have negative real parts if K is chosen in accordance with (47). Nevertheless, if any of the eigenvectors of A in the null space of C correspond to unstable modes, the original system will be unstable despite the fact that the cost J in (46) is unaffected. Consequently, if no stability problems are encountered, the above approach yields a solution to the optimal output feedback regulator problem for the original system as opposed to the optimal state feedback regulation.

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It is our opinion that these preliminary results reveal the great potential usefulness and versatility of the aggregated-system concept. The host of questions which can be raised when H is not an aggregate matrix and/or when dynamical feedback is permitted opens up a research area which we believe to be important and exciting, especially in view of our past experience in control.

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B. Enhancement, Extraction and Reconstruction Techniques

A. Papoulis and L. Kurz

1. Objective

The main purpose of this research effort is to investigate some new and promising approaches to the general problem of image enhancement, extraction, and reconstruction. The investigation will encompass two philosophically different classes of techniques: spectral-estimation and statistical.

In connection with the spectral-estimation approach, it is proposed to develop a new method of filtering, combining frequency domain techniques with the advantages of adaptive and recursive estimators. The method is based on the representation of an arbitrary signal $f(t)$ in terms of the samples of its "running FFT," and it can be used without any knowledge of prior statistics. A special form of the filter leads to an extension of the gradient-seeking algorithm used in a variety of LMS estimators. The study will include the development of the properties of running transforms and their use in spectral estimation.

The statistical class of techniques will include the study of several types of statistical masks, edge detection procedures, and image reconstruction algorithms. In addition, feature extraction and object identification based on various versions of factor analysis techniques will be studied.

The prime objective of the research effort is to obtain general results with broad implications in such areas as interpretation and classification of pictorial data, processing of radar data of all forms, geological and underwater sounding, meteorological and oceanographic data, space and communications data, etc. Whenever feasible, comparative studies of the two classes of approaches for a given application will be introduced.

Among others, the following aspects will be considered: various features of image processing with emphasis on noise and clutter reduction; detection of quasimonochromatic sonar signals in the presence of echoes and engine interference; rapid measurement of the instantaneous frequency of FM signals; adaptive equalizers; recursive estimation of covariance matrices.

2. Approach

The two different basic approaches are discussed separately in the presentation below.

(a) Spectral-Estimation Approach

To place the proposed spectral method into familiar perspective, we shall relate one of its applications to adaptive LMS estimation. We shall use as an illustration the estimation of a discrete process $y[n]$ in terms of the output (see Fig. 1)

$$\hat{y}[n] = \sum_{k=0}^{N-1} a_k[n] x[n-k] = X^T[n] A[n] \quad (1)$$

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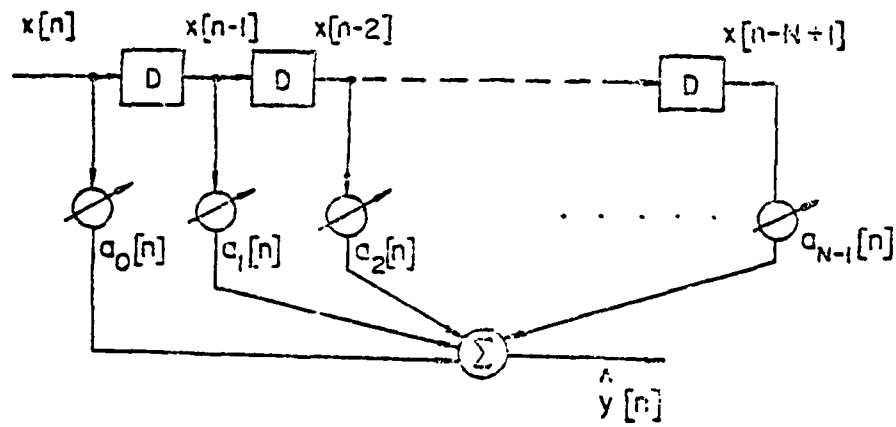


Fig. 1. Adaptive estimator.

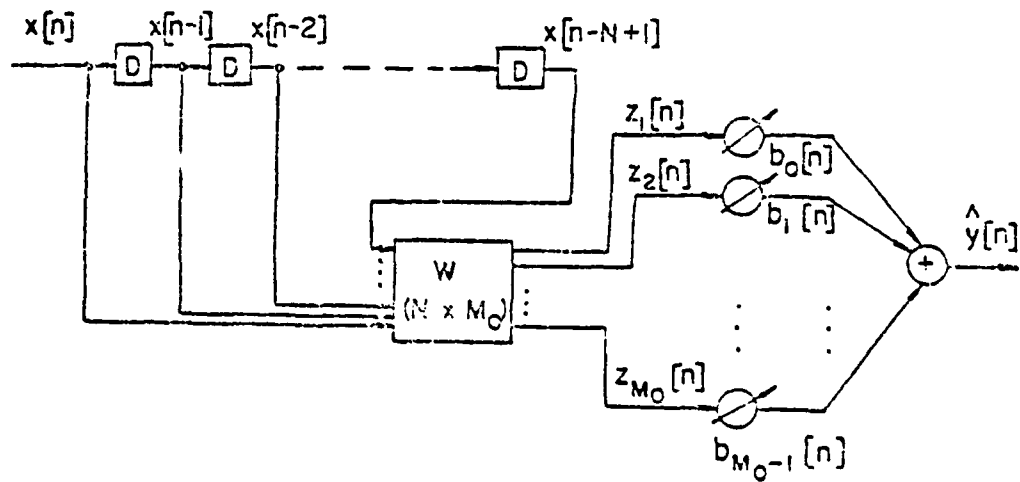


Fig. 2. Frequency domain adaptive estimator.

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of a non-recursive time-varying filter of length N with the data process $X[n]$ as the input. Our objective is to determine the weights $a_k[n]$ so as to minimize the MS value of the estimation error

$$e[n] = y[n] - \hat{y}[n] \quad (2)$$

If the statistics of the processes $x[n]$ and $y[n]$ are known, then (Wiener filter)¹

$$A[n] = R^{-1} \Gamma \quad (3)$$

where

$$R = E\{X[n]X^T[n]\} \quad \Gamma = E\{X[n]y[n]\} \quad (4)$$

In the absence of this information, we can either estimate the covariance matrix R and the cross-covariance vector Γ or we can determine $A[n]$ adaptively. A simple method of adaptation based on an instantaneous version of a gradient-seeking technique for minimizing the MS error is the algorithm

$$a_k[n+1] = a_k[n] + u e[n] x[n-k] \quad (5)$$

introduced by Widrow^{2,3} and used in several areas of signal processing.⁴

The Widrow filter is simple; it requires no prior knowledge of any statistics, and it can be applied to stationary and non-stationary processes. It has, however, a number of disadvantages: The number N of coefficients that are adaptively controlled equals the length N of the filter. This often introduces unnecessary complications if N is large. Filtering of noise is best performed in the frequency domain. This leads to a small number of unknown parameters if they control directly the frequency response of the filter. The filter of Fig. 1 does not have that property. The solution of (5) is a random set of weights $A[n]$ that does not approach the Wiener optimum^{5,6} [see (3)]. The estimation can be simplified if the adaptively controlled coefficients are associated with nearly uncorrelated data (Karhunen-Loeve).¹ This is not the case, in general, with the data $x[n-k]$ in (1). The length N of the filter is fixed; this is often undesirable.

To overcome these difficulties, we impose the restriction that the N weights $a_k[n]$ are linearly dependent on M_0 parameters $b_m[n]$:

$$A[n] = W B[n]$$

In the above, $B[n]$ is a vector consisting of M_0 elements and W is an $N \times M_0$ matrix to be determined. Inserting into (1), we obtain

$$\hat{y}[n] = X^T[n] W B[n] = Z^T[n] B[n] \quad (6)$$

where

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$$Z[n] = W^T X[n] \quad (7)$$

Equations (6) and (7) specify the system of Fig. 2, consisting of the matrix W transforming the N -vector $X[n]$ into the M_0 -vector $Z[n]$, followed by the M_0 weights $B[n]$ and an adder. The vector $B[n]$ is adaptively controlled:

$$B[n+1] = B[n] + u e[n] Z[n] \quad (8)$$

as in (5). However, unlike (5), we have only M_0 unknown weights and, as we shall see, M_0 can be much smaller than N .

The selection of the matrix W depends on the properties of the processes $x[n]$ and $y[n]$. Suppose, for example, that

$$x[n] = y[n] + v[n] \quad (9)$$

where $v[n]$ is noise. The vectors $X[n]$ and $Y[n]$ and elements $x[n-k]$ and $y[n-k]$, respectively are points in an N -dimensional space. If the signal vector $Y[n]$ belongs to a subspace S_y of dimensionality M_0 , then we choose for W the projection operator into S_y .

In the selection of W , we are guided by the following: small M_0 ; data vector $Z[n]$ with uncorrelated components; frequency domain properties of $Z[n]$. To meet these requirements, we select for W a matrix whose elements are the roots of unity:

$$W^{km}, \quad W = e^{j2\pi/N}, \quad 0 \leq k \leq N-1, \quad -M \leq m \leq M \quad (10)$$

where $M_0 = 2M+1$ and the index is suitably changed. The elements of the resulting vector $Z[n]$ are given by [see (7)]

$$F[n, m] = \sum_{k=0}^{N-1} x[n-k] W^{mk} \quad (11)$$

that is, they are the discrete Fourier series (DFS) of the N samples $x[n], \dots, x[n-N+1]$ of the input $x[n]$.

With this choice of W , the output of the filter of Fig. 2 is given by [see (6)]

$$\hat{y}[n] = \sum_{m=-M}^M b_m[n] F[n, m] \quad (12)$$

and the coefficients $b_m[n]$ are adaptively controlled:

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$$b_m[n+1] = b_m[n] + u_m e[n] F[n, m] \quad (13)$$

In the next section, we present preliminary results concentrating on the properties of running transforms. The material is developed for simplicity in one dimension.

(b) Various Statistical Approaches

The masking techniques and techniques based in ANOVA (analysis of variance) used by the senior investigator (Professor Kurz) in the past may be unified within the framework of the statistical linear models. In a recent paper,⁷ he introduced a collection of simple procedures based on masks to be used in computer image processing. Small, carefully selected regions of an image are viewed at one time. The process is repeated throughout the image. Many different types of masks were introduced which accomplish efficiently the tasks of edge detection, noise reduction, shrinking, expansion, object recognition, measurement, etc. In a separate paper⁸ the effectiveness of ANOVA techniques were demonstrated in image processing and enhancement. Simultaneously, classes of Robbins-Monro type stochastic approximation minimum variance least squares (SAMVLS) estimators were developed^{9,10,11} for which the resultant regression function is interpreted as a recursive correlator. Robustness (relative insensitivity) to variations distribution and insensitivity to contamination of data) is achieved by batch preprocessing of the data either by using linear rank tests (batch-nonlinear-linear or BNL approach) or by using adaptive gain coefficients with properly preselected nonlinearity. By combining the theory of ANOVA, experimental design and robustized SAMVLS, new three-dimensional recursive masks may be introduced for real-time parallel processing and detection of stationary or moving images in unspecified noise environment from observations taken of a noisy scene. The method has the potential for development of techniques for estimation of velocity and acceleration of moving objects. In addition, the theory of Latin Square experimental designs is particularly attractive as an approach to the design of three-dimensional masks.

In a separate paper,¹² it was demonstrated that two-dimensional partition tests are effective in achieving excellent quality edge detection in the presence of severe and undeformed noise. The Philosophy of this approach needs further extension to include nonlinear processing which is particularly useful in the processing of images appearing in radar and underwater sounding data. The extended model will include the problem of moving objects, velocity, acceleration, etc.

Using masking techniques in conjunction with occupancy vectors of partition tests represents an interesting marriage of the two approaches outlined above. The full impact of this hybrid version of image processing problems is not clear at this time but preliminary results indicate its potential for efficiently solving numerous problems in image processing.

The SAMVLS algorithm mentioned above¹¹ permits one also to attack the problem of image reconstruction. Preliminary results in this area are available

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in reference 13. The preliminary results of this approach are promising and justify a major effort in this area.

Two classes of recursive factor analysis techniques as means of achieving feature extraction and image identification were introduced in Reference 14. This approach is particularly useful in processing massive arrays of data. Further development and refinement of this approach will result in the attainment of an efficient software library for reducing and identifying severely corrupted and/or unknown images embedded in an unknown background noise.

3. Progress

Progress will be reported separately for the spectral estimation and statistical approaches.

- (a) We concentrated on the following: estimation of various classes of stationary and non-stationary processes using adaptive frequency domain filters and comparison with other methods. Properties of the running transforms of deterministic and random signals. The results were presented in two conferences and led to several papers.

Conferences:

1. "Adaptive Frequency Domain Estimators," IEEE International Symposium on Information Theory, June 25-29, 1979, Grignano, Italy.¹⁵
2. "Spectral Estimation from Random Samples," International Conference¹⁵ on¹⁶ Information Sciences and Systems, IEEE and Univ. of Patras, Greece, July 1979.

Papers:

3. "Detection of Hidden Periodicities by Adaptive Extrapolation," IEEE Transactions on Acoustics, Speech and Signal Processing, to appear October 1979.⁸
4. "Adaptive Frequency Domain Filtering and Estimation," IEEE Transactions on Information Theory, submitted for publication.¹⁷
5. "Theory and Applications of Running Transforms," IEEE Transaction on Circuits and Systems, submitted for publication.¹⁸

To give an indication of the effectiveness of the method, we show below a typical application in a prediction and filtering problem and compare the solution with the solution obtained using a Widrow filter. The problem under consideration is the estimation of the future value $s[n+1]$ of a discrete signal in terms of the N most recent values

$$x[n], x[n-1], \dots, x[n-N+1] \quad (14)$$

of the sum (Fig. 3)

$$x[n] = s[n] + v[n] \quad (15)$$

where $v[n]$ is additive white noise. The signal $s[n]$ is a stationary discrete process generated on the output of a fifth order Butterworth filter $H(s)$ driven by white noise $z[n]$.

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The Widrow estimator is shown in Fig. 4. Its output $\hat{y}[n]$ is the sum

$$\hat{y}[n] = \sum_{k=0}^{N-1} a_k[n] x[n-k] \quad (16)$$

requiring N adaptively controlled coefficients $a_k[n]$. The adaptation algorithm is the first order recursion

$$a_k[n+1] = a_k[n] + \mu \{s[n+1] - \hat{y}[n]\} x[n-k] \quad (17)$$

the results are shown in Fig. 2 for $N = 32$.

Adaptive filtering based on running transforms is shown in Fig. 5. The results one obtains with $M_0 = 1$. Thus, using only $2M_0 + 1 = 3$ adaptively controlled parameters, we obtain a prediction that is as efficient as the time-domain prediction requiring $N = 32$ adaptively controlled parameters.

- (b) In connection with the work on statistical approaches to the problems of image enhancement, extraction and reconstruction, several important results were obtained during the past year.
- (1) The ill-posed problem of object reconstruction was reformulated in the framework of the general linear model in a new recursive parametric form.^{19,20} The resultant algorithms were shown to be natural stabilizers of the inherent instabilities of both the iterative and non-iterative reconstruction methods. Both robustized and unrobustized versions of the algorithms were given. The recursive algorithms provide immunity to measurement noise outliers in burst noise of high variance. Unlike procedures suggested previously, these methods eliminate the need for stopping rule constraints and ensure convergence of the algorithms in the mean-square sense and with probability one. The recursive formulation of the non-iterative method has broad implications to the problem of restoration of multidimensional images.
- (2) The theory of the linear hypothesis model, ANOVA, experimental designs and robustized Stochastic Approximation Minimum Variance Least Squares (SAMVLS) were united and applied in a pattern recognition framework to edge element detection and enhancement of large arrays of three-dimensional pictorial data.²¹ New Three-Dimensional Recursive Parallelepiped Masks (TDRPM) suitable for real-time parallel processing and detection of stationary and moving edge elements were developed from multiple pictures taken of a scene in unspecified noise. The TDRPM were implemented by SAMVLS as a $2 \times 2 \times k$ and ANOVA as a $2 \times 2 \times 5$ mask. The concept of Relative Sensitivity Efficiency (RSE) was introduced to allow comparisons with larger two-dimensional mask. Extensive computer simulations demonstrated the successful performance of TDRPM either as a stationary or a moving edge detector.
- (3) The theory of Latin Square experimental designs was extended to include edge detection of multi-grey level pictorial data.^{22,23} Latin Square designs were realized using mask operations either as a square or in linear forms using ANOVA to estimate the model parameters. The test statistics are based upon the robust F -test and the thresholds are selected by an empirical interactive

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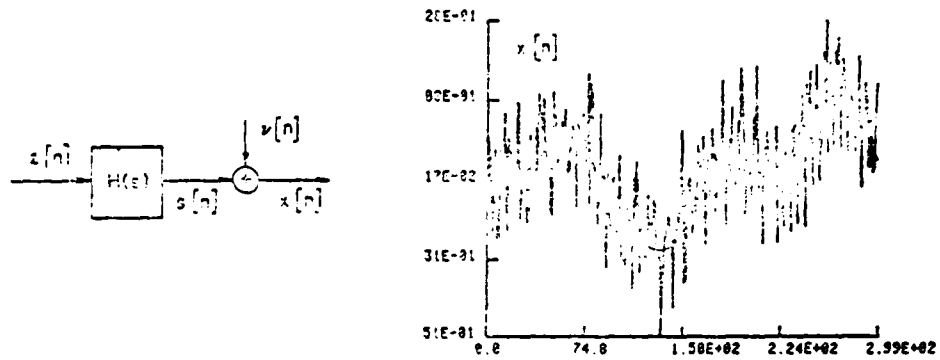


Fig. 3. The noisy signal and the signal.

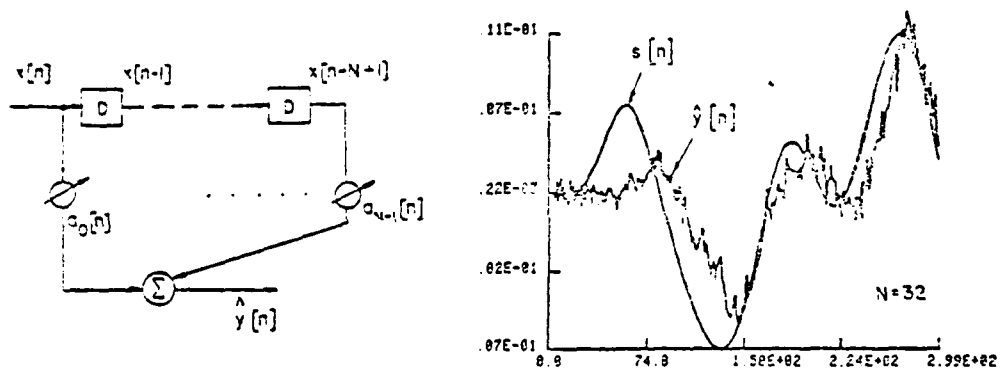


Fig. 4. Widrow filter output.

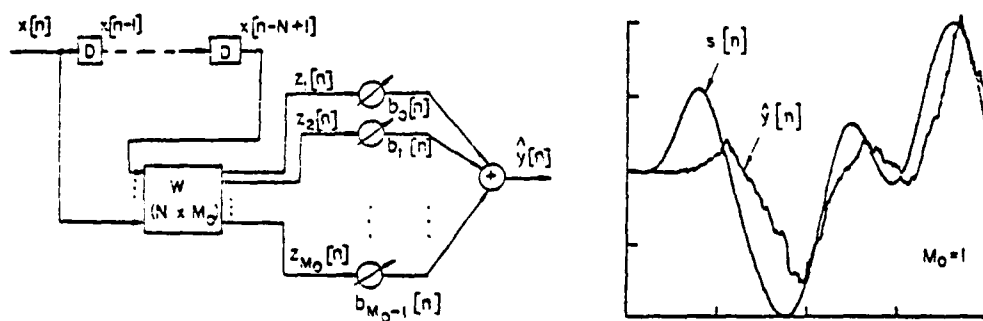
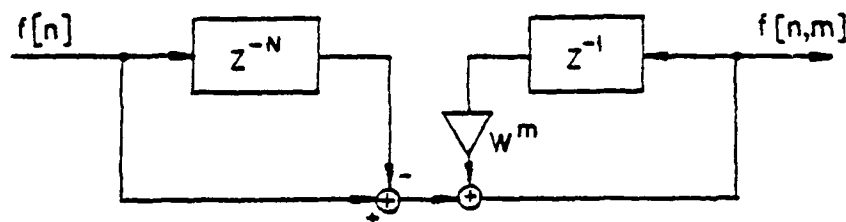


Fig. 5. Two terms are updated in the frequency-domain Widrow filter.

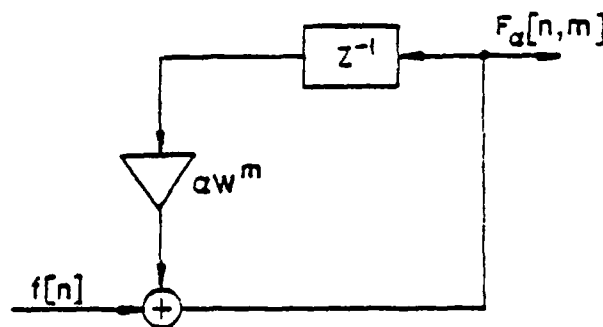
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process. A post hoc comparison method is used to confine the edge element ambiguities to two-pixel layer thickness in masks greater than 2×2 pixels. The theory was verified by computer simulations.

- (4) The edge detection problem in multilevel images under moderate and high signal-to-noise ratio conditions has been treated by many authors. If images are severely corrupted by noise, the procedures suggested in the past do not perform satisfactorily. A new quadratic m -interval test was developed to endure an efficient M -grey level detection of image edges severely corrupted by noise.²⁴ The procedure was verified by application to simulated data.
- (5) In most procedures used for image detection or enhancement, the measure of performance of a given procedure is usually based on empirical methods, asymptotic analyses and/or simulation studies. As an alternate approach, a bound on the probability of image misclassification based on the two-dimensional inequality was introduced.⁴⁵ The parameters in the inequality are obtained from appropriate simulation studies.



(a) DFS analyzer.



(b) Modified DFS analyzer.

Fig. 6

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C. Robust Procedures in Estimation and Detection Problems

L. Kurz

1. Objective

Considerable interest generated in robust estimation and detection problems motivated the development in recent years by the senior investigator in cooperation

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with his doctoral students of several classes of rank and non-rank detection procedures as well as robust estimation procedures which use nonparametric preprocessors to achieve a high degree of robustness in the presence of unknown noise and/or severe extraneous contamination of the data. The main objective of future research is to concentrate the effort on classes of detectors based on mixed statistics which preserve excellent qualities of rank and non-rank procedures; also included in the effort will be the imposition of side constraints, statistical dependence, sequential modes of operation and array processing of the data. A parallel effort will include extensions of the robustized estimation techniques to problems involving stochastic approximation minimum variance least squares estimators (SAMVLS) and Kalman-type estimation and filtering problems. The interaction of the robust detection and estimation techniques in adaptive systems will be studied. Particular attention will be given to the application of the procedures to problems in radar, sonar and communications.

2. Approach

The statistical properties of partition detectors and their variants are well understood. A concise exposition of the present state of the art may be found in Reference 1. The mathematical framework introduced therein permits a logical evolution of many robust detectors with an almost inexhaustible source for developing such detectors useful in various applications. In addition, two approaches introduced in a recent paper of ours² for including side constraints in the design of robust detectors represent a major step in our ability to evolve many flexible procedures for robust detection subject to various physical constraints. Inclusion of statistical dependence and sequential modes of operation^{2,3,4} adds another important dimension to the utility of partition detectors. The interaction of the approaches outlined above represents an almost inexhaustible source for solving numerous interesting and useful problems involving detection of weak signals in an unknown environment.

In a recent paper,⁵ a new class of non-rank robust detectors, which are related to the generalized quantile detector¹ was considered. Unlike the non-rank detectors based on quantile statistics with fixed scoring vectors, the new class of detectors uses a random scoring vector. This new class of detectors is particularly useful in a noise environment that is relatively rapidly varying.

The approach to robust recursive estimation problems initiated in References 6 and 7 with its extensions presented in References 8 and 9 represents another source of numerous theoretical and practical problems of interest in radar, sonar and communications. Inclusion of statistical dependence and other constraints in this approach will yield a tool of almost limitless potential for solving practical estimation problems when the parameters to be estimated are severely corrupted by noise or the noise is unknown or varying. Various additional forms of robustized estimators, including p.d.f., c.d.f., and score estimators, permit solution of numerous practical problems. For all approaches outlined above stress will be placed on procedures which are applicable in real-time processing and are simple to implement.

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3. Progress

- (a) The problem of statistical dependence on partition detectors² was extended to sequential detectors.¹⁰ In particular, a new formulation was introduced which predicts the thresholds under q -dependent sampling in order to maintain the same error probabilities as in the independent sampling case. A comparison is made between independent and dependent sequential partition detectors based on the average time to detection. Under stated conditions, dependent sequential partition detectors show improved efficiency for both Lehmann and shift of the mean alternatives.
- (b) The sequential partition detector (SPD)³ was compared with two sequential non-parametric detectors developed by Chadwick and Kurz.¹¹ Two important results should be stressed: (1) The SPD has the advantage of being able to specify α , β , and adjusting ASN by varying signal strength in advance, whereas it is not possible to do so for detectors of reference 11; (2) by increasing¹² the number of partitions, m , the SPD represents a generalization of the sequential sign test of reference 11.
- (c) An important problem in radar and sonar is the detector of sinusoidal signal in noise. Busgang and Middleton¹³ obtained the optimum sequential test for the envelope of narrow-band noise and an additive sine wave. Blasbalg¹⁴ obtained the optimum "slicing threshold" for a Bernoulli sequential detector operating under a sine wave carrier in zero mean Gaussian noise. For this model we found that the optimum threshold corresponded to 65 percent efficiency of the detector. If the theory of sequential partition detectors³ (SPD) is applied to the model of reference 13, one can obtain the same performance efficiency in small S/N environment as in reference 14 for $m=2$, but the robustness of the SPD is superior. If the number of partitions, m , is increased to 10, the efficiency of detection reaches 97.7 percent while preserving the robustness of the SPD.¹⁵ For large S/N, the ASN of the optimum and SPD detector are essentially the same for $m > 4$.
- (d) Contributions of large amplitudes of impulsive noise to the test statistic corresponding to SPD may reduce the effectiveness of its robustness. In this situation, the performance of the detector may be improved by introducing regions of large signal ambiguity by setting two upper thresholds in the detector.¹⁵ The thresholds may be fixed or variable. For all forms of thresholds the performance of SPD is significantly improved in the presence of impulsive noise accompanied by an insignificant increase in ASN.
- (e) The theory of robustized stochastic approximations of Gladyshev's form was extended to the vector form.¹⁷ Two applications of the procedure were investigated so far - estimation of parameters in a linear model¹⁷ and a robustized vector recursive stabilizer algorithm for image restoration.¹⁸ Other applications of the theorem are subject to future investigation.

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SECTION IV: SIGNIFICANT ACCOMPLISHMENTS

1. A Novel Acoustoelectric SAW FM Demodulator

W-C. Wang, H. Schachter and F. Cassara

We have invented and successfully constructed and tested a novel acoustoelectric FM demodulator. A phenomenological theory to describe the principle of operation has also been successfully developed. Experimental results are in close agreement with the theory.

This new type of demodulator possesses a number of unique features over conventional demodulators. It is first of all of particularly simple configuration, consisting only of two identical transducers and a thin semiconductor plate placed directly on a piezoelectric substrate. Although designed and tested at 100 MHz, it is capable of operating at a high carrier frequency, perhaps 1 GHz, and it is expected to be capable of accommodating wideband signals with deviations up to 20 MHz, sufficient for analog FM signals as well as high speed digital data. A unique feature is that it can be designed to either recover the modulating signal or detect its second harmonic by simply introducing a frequency offset in the received carrier.

The frequency-modulated input signal is applied simultaneously to two identical SAW transducers separated by a small distance. The resulting two co-linear surface acoustic waves are thus propagating in the same direction with a time separation specified by the distance between the transducers. The two waves are then passed under a semiconductor plate placed on the piezoelectric substrate. In the experiment, we used a Si plate on a LiNbO_3 substrate. When the two waves propagate under the semiconductor, the piezoelectric field associated with the waves will induce space charge waves inside the semiconductor. Through the nonlinear interactions among the induced space charge waves and the piezoelectric field waves, many higher-order signals are generated, but, after integrating along the semiconductor length, it can be shown that only the term which performs FM demodulation is of significant amplitude, and can be detected across terminals which are placed at the front and back ends of the semiconductor plate. Furthermore, since the operation is based on the tangential component of the electric field, and not the normal component, it is not necessary to employ an air gap between the semiconducting plate and the substrate; the device is thus less critical in construction than a convolver.

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2. The Interaction of Currents, Charges, and Strains in the Surface Regions of Metals

H. J. Juretschke

It has been known for over seventy years that an electrostatic charge distribution placed on the surface of a metallic conductor can change the metal's electrical conductance. Despite quite a few attempts at definitive experimentation over the years, and various theoretical proposals, the causes of this effect have remained obscure. It is a small interaction - limited mostly by the maximum surface charge density a metal can acquire before there is electrical breakdown of the region above its surface - but it has remained of interest because it represents one of the few manifestations of a metal's time-independent deviation from local charge neutrality. More recently, it has attracted additional attention as a possible probe for exploring the surface regions of metals. Since in most good metals the electric fields of static surface charges are screened within a depth of less than one atomic layer, these fields should disturb only the outermost surface region and its properties.

As a result of our own investigations of this phenomenon, the so-called Metallic Field Effect, we believe that we now understand what is most likely the dominant mechanism by which a static surface charge density q influences the electrical transport in metals. When an external electrical field terminates on surface charges, it is accompanied by normal and transverse Maxwell stresses proportional to q^2 . In addition, theory predicts that a solid will generally also sustain a surface stress proportional to q . These q -terms and q^2 -terms correspond, respectively, to surface piezoelectricity and electrostrictive effects, both allowed because of the reduced structural symmetry of the surface region. Both kinds of stresses can cause elastically reacting strains in the solid; the magnitude and extent of these strains are governed by the elastic properties of the solid, of the region above the solid, and of the coupling between the two within the interface. In general, therefore, electrostatic charging of the surface is accompanied by strain fields that extend into the metal over distances large compared to the direct screening depth of electric fields.

We have established that it is the scattering of current carriers by these strain fields which gives rise to the phenomena observed in the Metallic Field Effect, at least in the standard configuration of a thin metal film adhering rigidly to a dielectric. Here the q^2 -strains extend throughout the film thickness,

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and they can be ascribed quantitatively to a change in film conductance using the known elastoconductive sensitivity of metals. The q-strains, restricted to the interface region - and for these there exists no detailed theory - are now known to produce a change in conductance via the same mechanism, as established largely through the overwhelmingly analogous features of both contributions to the Metallic Field Effect at the surfaces of ferromagnetic metals. All numbers deduced from the experiments have plausible magnitudes.

These conclusions were not anticipated by any theoretical models. They suggest that the coupling between electric and strain fields at a metal surface is a feature of most materials, and that the new topics of surface piezoelectricity and electrostriction are accessible to detailed examination. This may reveal additional new phenomena. Furthermore, since the range of the strain fields below the surface can be controlled by adjusting the elastic boundary conditions, the Metallic Field Effect will lend itself to probing the metal to different depths below the surface. Conversely, it is expected to be sensitive to any boundary conditions imposed by surface treatments, such as for example oxidation, on the elastic, and therefore now also on the electrical, response of the surface region of metals. Finally, with known strain fields, we can learn more about the characteristic scattering mechanisms of charge carriers in this region.

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3. A New Class of Leaky Modes on Open Dielectric Waveguides

S. T. Peng and A. A. Oliner

Last year we found that under appropriate conditions certain modes of dielectric strip waveguides for integrated optics¹ and for millimeter waves are leaky instead of being purely bound. This year we have obtained an understanding of the process which is quite general and from which we can make predictions relating to various classes of waveguides; we can determine which classes of guides may leak and which never leak, which modes will do the leaking and which will not, and we can prescribe how to modify the waveguiding structure to avoid leakage, or alternatively to produce leakage when we wish to. In addition, we have developed a generally-applicable systematic but simple criterion² to determine when leakage will be present without having to first solve the specific problem.

It is important for two reasons to know whether or not leakage is present. Since open dielectric waveguides, whether at optical or millimeter wave frequencies, are intended for use in an integrated circuit fashion, unwanted leakage can cause cross talk between neighboring components and thus deteriorate the performance of the circuit. On the other hand, novel components can be designed which make deliberate use of the leakage present. An example of such a component for integrated optics is a novel leaky wave directional coupler.³ This coupler consists of the usual two strip waveguides located parallel to each other and spaced a certain distance apart, but here the spacing is made so great that the coupling would be negligible if leakage were not present. It is found that the coupling is not sharply sensitive to the separation between the strips, a feature which may have practical import. Of even greater interest is the coupler's potential use as a mode stripper or purifier. In general, when one wants to excite the TE mode on the optical strip guide some amount of TM mode energy will inevitably be present. Since the lowest TM mode on the optical strip waveguide leaks and the lowest TE mode does not, such a leaky wave coupler can be used to tap away all the TM mode energy without disturbing the TE mode at all.

Open dielectric waveguides can be broadly divided into two classes: those which are essentially modifications of dielectric rods, and those which are formed by a dielectric strip perturbing a planar dielectric waveguide. Examples of the first class are the dielectric image line for millimeter waves, a dielectric strip placed on a dielectric substrate, and a channel diffused or

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implanted into the surface of a dielectric substrate, the latter two arising in integrated optics. Examples of the second class are the "insular" guide and the inverted strip guide for millimeter waves, and the dielectric strip guide, the rib guide, and the slot guide for integrated optics. In all examples of the second class, the waveguide has dielectric wings, that is, a wide planar dielectric layer is present which could guide a wave in the absence of the central strip which concentrates the field. All waveguides falling into the first class possess only purely bound modes; none of the modes are ever leaky (assuming that the waveguide is longitudinally uniform, of course; a taper or appropriate periodic loading will produce leakage). On the other hand, leaky modes can be present on waveguides of the second class. But even here, broad distinctions can be made; for example, the "insular" guide will never leak, but the inverted strip guide will usually leak. It is also interesting that indiffused channels, which fall into the first class, are sometimes fabricated with wings⁴ to enhance coupling between neighboring structures. They thus fall into the second class, and this fact may explain some of the anomalous behavior⁴ associated with them.

The leakage, when it occurs, is due to the coupling between the constituent TE and TM waves produced at the strip sides when these waves bounce back and forth in the strip region, as part of the guiding process. The general criterion referred to earlier requires one to investigate the dispersion behavior for the independent TE and TM waves in each of the constituent regions in the waveguide cross section, assuming each region to be infinitely wide. On those structures which may leak, it is found that the lowest mode never leaks, the next mode (which is usually present simultaneously) may or may not leak depending on the geometric conditions, and modes formed from the higher modes in the planar dielectric layer almost always leak. In predictions, care must be taken to determine which mode, in fact, is the lowest mode. For example, in the inverted strip guide for millimeter waves, it has been assumed that the TM mode, which is the incident mode, is the lowest one under customary operating conditions; in fact, a cross-over occurs, and the lowest mode is really the TE mode, with the result that the TM mode leaks, contrary to expectations.

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